SMART X2S

- User Manual

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Innovation with Integrity

SC-XRD

This document covers the SMART X2S system.

References to this document should be shown as DOC-M86-EXS127 SMART X2S User Manual.

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Address comments to:

Technical Publications Department
Bruker AXS Inc.
5465 East Cheryl Parkway
Madison, Wisconsin 53711-5373
USA

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Bruker Corporation

40 Manning Road
Billerica, MA USA

Phone +1 (978) 663-3660
Fax: +1 (978) 667-5993

E-mail: info@bruker.com
www.bruker.com

Bruker AXS Inc.

5465 East Cheryl Parkway
Madison, WI 53711-5373 USA

Phone +1 (800) 234-XRAY [9729]
Fax +1 (608) 276-3006

E-mail: info@bruker-axs.com
www.bruker-axs.com

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1 About this User Manual

1.1 The Structure of this User Manual

This User Manual describes the SMART X2S and its functions, and illustrates the steps required to perform a structure determination:

- **Introduction to the SMART X2S** describes the system, its specifications, and its functions;
- **Sample Preparation and Mounting** discusses separating a crystal from the bulk sample and attaching it to the micromount;
- **Setting Up Data Collection** starts the data collection by entering crystal information, and then inserting the blank CD and sample;
- **Data Collection and Structure Solution** describes the steps in the SMART X2S automatic data collection and structure solution phase;
- **Structure View, Report Display, and CD Burning** describes the SMART X2S results after collecting and solving the structure;
- **The Data CD** describes the report and files on the CD, which contain all the information necessary to publish the structure (or, if desired, work further with it in Bruker's APEX2 software suite); and
- **SMART X2S Administrator Information** discusses procedures and operations to be carried out by the SMART X2S Administrator (i.e., an on-site person responsible for the instrument's security, safety, and function).

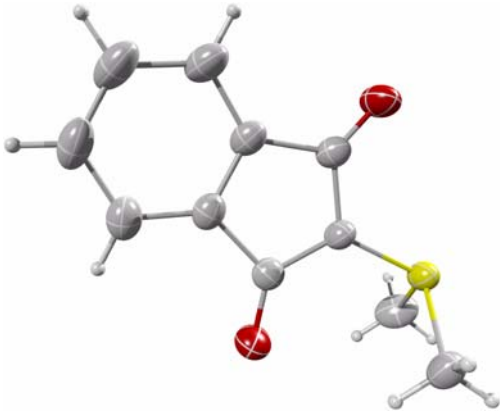
1.1.1 The Ylid Crystal

The compound used was 2-dimethylsulfuranylidene-1,3-indanedione (abbreviated “ylid”):

$C_{11}H_{10}O_2S$

More information on the ylid crystal is available in the article “Polymorphism and History of 2-Dimethylsufuranylidene-1,3-indanedione (YLID)”, Ilia A. Guzei, Galina A. Bikzhanova, Lara C. Spencer, Tatiana V. Timofeeva, Tiffany L. Kinnibrugh and Charles F. Campana. *Cryst. Growth Des.*, **2008**, 8 (7), pp. 2411–2418, DOI: 10.1021/cg701260p.

Figure 1.1 — Ylid crystal structure



1.2 Referenced Documentation

The following Table contains a list of documentation referenced by this document. It is necessary to have this additional documentation available as you work with this document. In the documents’ part numbers, a variable revision number is indicated by a letter “X”. Always use the most current revisions available.

All of the documents shown in the Table may be found at Bruker AXS’ comprehensive support site www.brukersupport.com, or on the Online Documentation CD-ROM that accompanies the shipment.

1.2.1 Referenced Documentation

Table 1.1 — Referenced documentation

Documentation Part Number	Title
A86-Exx003	Fundamentals of Single-Crystal X-ray Diffraction
M86-Exx078	APEX2 Software User Manual (if applicable)

1.3 Terms and Conventions

1.3.1 Equivalent Terms

Frame/Image

In 2-dimensional X-ray diffraction, the terms *frame* and *image* refer to the same 2-dimensional view of the diffraction pattern.

Greek and Roman Text

This document uses scientific terminology that may be rendered in Greek text. However, this document follows a convention of using Roman text to the greatest extent possible.

Table 1.2 — Greek and Roman Text

Greek	Roman
2θ	2theta
ω	omega
φ	phi
χ	chi

1.3.2 Notices: Danger, Caution, and Note

This document contains notices that must be observed to ensure personal safety, as well as to protect the product and connected equipment. These notices are highlighted as follows according to the level of danger.

DANGER

The word “DANGER” alerts you to an immediate or potential hazard that can result in death, severe personal injury, or substantial property damage.

CAUTION

The word “CAUTION” alerts you to a potential practice or condition that could result in minor personal injury or damage to the product or property.

NOTE: The word “NOTE” in bold capital letters draws your attention to particularly important information on the product or handling of the product, or to a particular part of the product documentation.

1.4 Safety Notices

1.4.1 General Safety Precautions of the SMART X2S

DANGER

X-ray Radiation!

The SMART X2S is an analytical instrument with a strong X-ray source. Shielding and safety equipment guarantee that the emitted radiation does not exceed 1.0 µSv/h during operation.

Shielding and safety features designed into the equipment guarantee that the emitted radiation does not exceed 1.0 µSv/h (at 5 cm from any external surface of the device) during operation. This level is below the regulatory limit in all jurisdictions. The ICRP dose limits in Publication 60 and 103 to the whole body for a radiation worker averaged over a 5-yr period is 20 mSv in a year, and for a member of the public it is 1 mSv in a year. It is highly unlikely that the radiation worker dose limits will be exceeded when trained and qualified personnel use such devices.

Read Section 1.4.4 X-ray Safety before turning on the system. Please observe local regulations for the operation of X-ray systems.

If you suspect that the safety system does not work correctly or that radiation protection is impaired for any reason, immediately switch off the system and contact your local Bruker AXS Service Representative. Manipulations and modifications of the safety systems are strictly forbidden!

NOTE: The X-ray generator is controlled by a two position Keyed switch (OFF/ON) similar to the ignition switch of a car. The key can only be removed when the switch is in the OFF position. The switch will remain in the OFF position until the key is inserted and turned. **Therefore the removal of the key will terminate production of X-ray.**

1.4.2 Correct Usage of the SMART X2S

The SMART X2S is intended for benchtop use only.

The SMART X2S may only be used for the applications specified in its User Manual or Specification Sheet, and only in conjunction with devices or components from other manufacturers that have been approved or recommended by Bruker AXS.

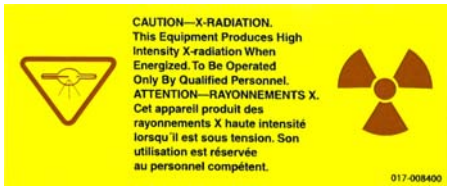
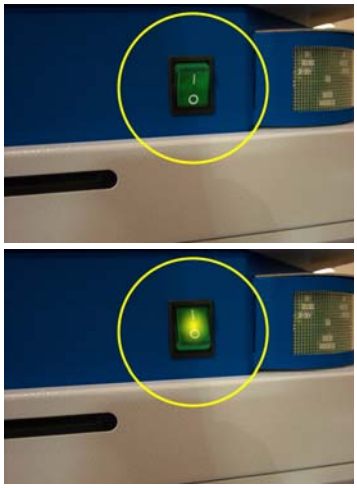
CAUTION

This product can only function correctly and safely if it is transported, stored, set up, and installed correctly, and if it is operated and maintained as recommended by Bruker AXS. If the SMART X2S is used in a manner not specified by Bruker AXS, the system's safety features may be impaired.

1.4.3 Safety-related Graphic Symbols

The safety-related graphic symbols on the SMART X2S chassis need to be fully understood before using the unit.

Table 1.3 — Safety-related graphic symbols

Symbol	Meaning
	The radiation warning label contains two internationally-recognized warning symbols, with descriptive text in English and French.
	The power switch uses the two icons “0” and “1” to describe the state of the switch. When the switch is off (i.e., “0” is in the depressed position), no power is being supplied to the SMART X2S. When the switch is on (i.e., “1” is in the depressed position), power is being supplied to the SMART X2S and the switch is illuminated green.
	The SMART X2S’ left and right radiation warning displays each contain two illuminated trefoil radiation symbols. When the X-ray generator is active (but the shutter is closed), an orange radiation symbol appears on each of the left and right displays. When the shutter is open, an additional red radiation symbol appears on each of the left and right displays.

1.4.4 X-ray Safety

DANGER

X-ray equipment produces potentially harmful radiation and can be dangerous to anyone in the equipment's vicinity unless safety precautions are completely understood and implemented. All persons designated to operate or perform maintenance on this instrument must be fully trained on the nature of radiation, X-ray generating equipment, and radiation safety. All users of the X-ray equipment are required to accurately monitor their exposure to X-rays by proper use of X-ray dosimeters.

For safety issues related to operation and maintenance of your particular X-ray generator, diffractometer, and shield enclosure, please refer to the manufacturer's operation manuals or to your Radiation Safety Officer. The user is responsible for compliance with local safety regulations.

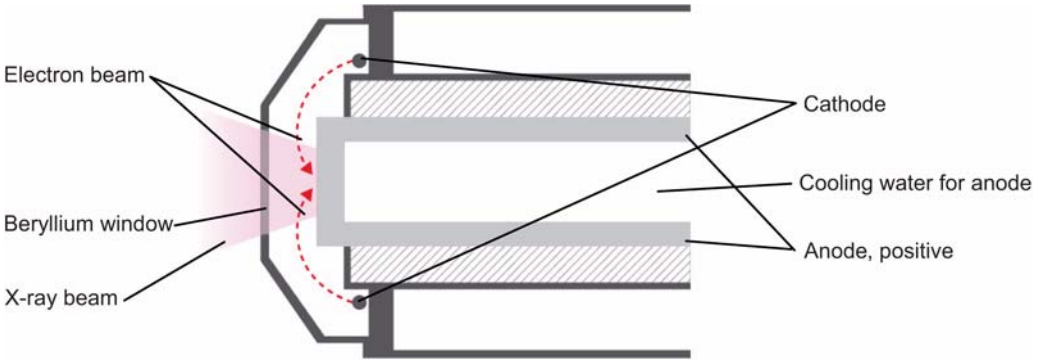
General Physical Principles of X-rays

Production of X-rays

X-rays are photons that are emitted when electrons strike a metal target and interact with the electrons orbiting the nuclei of the metal atoms. The electromagnetic waves in the λ range 0.1-2 Å are emitted in all directions.

In X-ray tubes, electrons are emitted by a heated cathode, accelerated, and strike an anode material. The cathode consists of a tungsten filament. For the generation of X-rays, high voltages of 20-60 kV are required. Much of the energy supplied to the tube is transferred to heat, while less than 1% of it is converted into X-rays. The anode consists of a metal (for example, Cu, Mo or Cr) that produces a characteristic wavelength. A water cooling system prevents it from overheating. X-ray tubes usually have a thin beryllium window by which the X-rays escape to the outside. The tube is partly clad with a heavy absorbing material (such as lead) to prevent the X-rays emitted in other directions from penetrating to the outside.

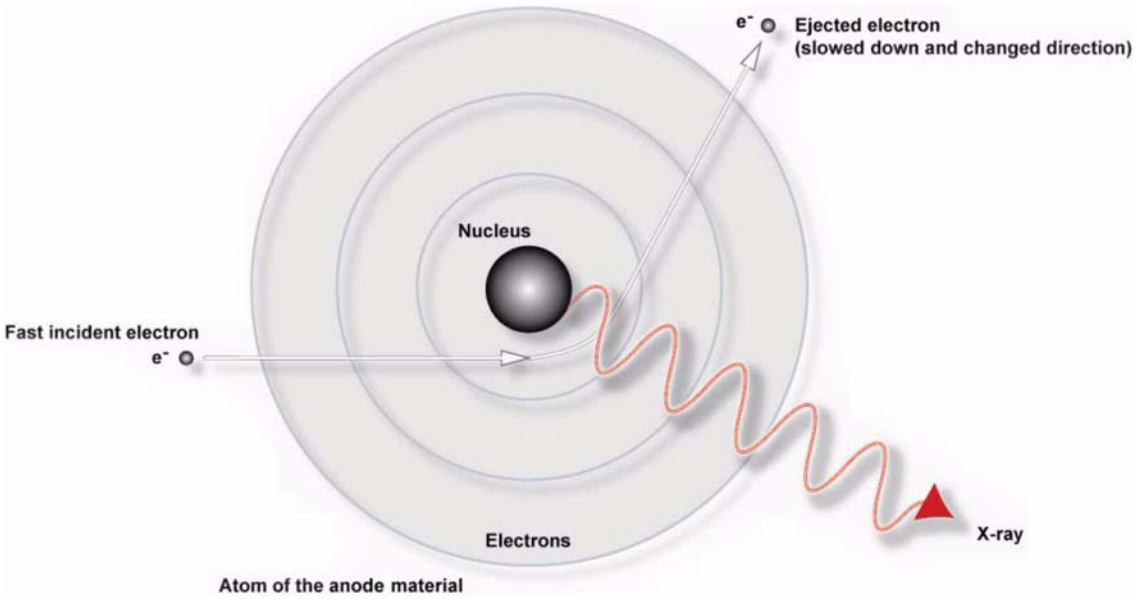
Figure 1.2 — Schematic diagram of an X-ray tube



Continuous Spectrum

When accelerated electrons collide with atoms in the metal target, they can be stopped on impact (in which case all their energy is converted into radiant energy), or they can be decelerated in steps (in which case a part of their total energy is released in the form of X-rays of greater wavelengths at each step until it is expended). The incident electron enters the electric field between the electrons and the nucleus of an atom and is deflected and decelerated by it at the same time. This process is repeated when the deflected electron enters the electric fields of other atoms.

Figure 1.3 — Production of continuous (white) radiation



The waves of X-rays generated in this way are called “continuous” radiation because they form a continuous spectrum of wavelengths.

Characteristic Spectrum

High-energy electrons can also interact with the atoms of the metal target to produce another type of radiation called “characteristic” radiation because the wavelengths of the photons emitted are characteristic of the anode metal.

In this case, the incident electron collides with an electron of the first, innermost electron shell of an atom and knocks it out of its orbit. To restore stability to the energy state of the atom, the ejected electron is replaced by an electron from an outer shell. Because the energy levels of shells increases with their distance from the nucleus of the atom, the transition of a replacement electron from an outer to an inner shell is accompanied by a loss in energy, which is released in the form of X-rays.

Figure 1.4 — Production of characteristic radiation (simplified representation)

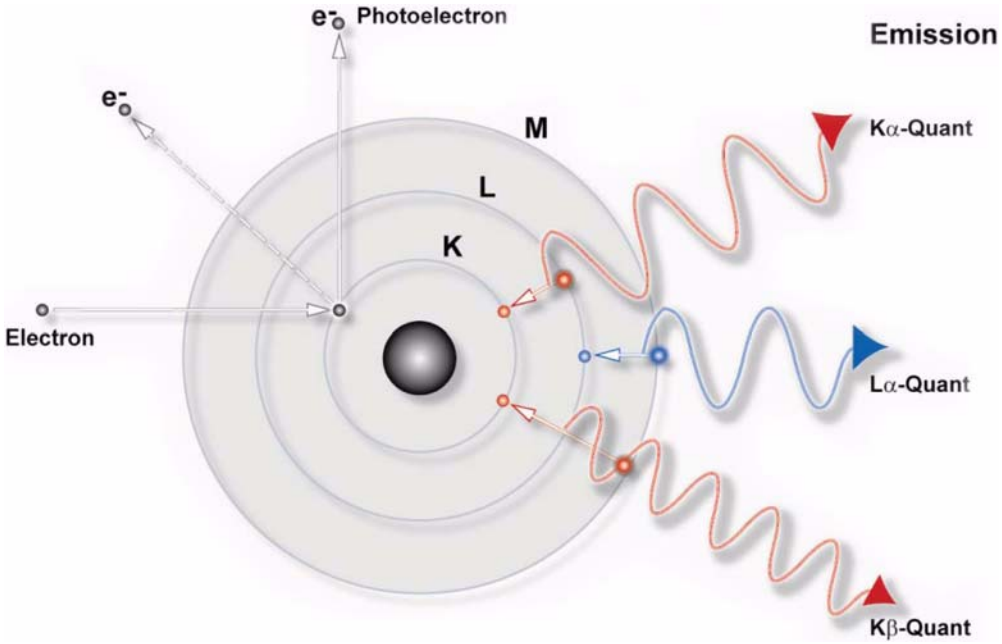
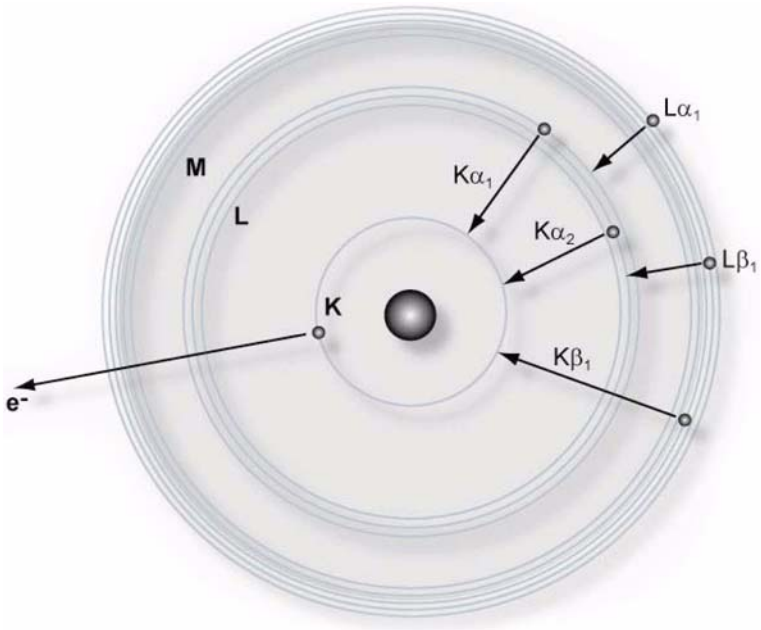


Figure 1.4 is a simplified representation of the process by which characteristic radiation is produced through the transition of electrons at the atomic level. In this diagram the conventional notation for the electron shells and the photons produced by the transition of their respective electrons has been adopted. Kα radiation is produced by an electron transfer from shell L to shell K, Kβ by a transfer from shell M to shell K, and Lα by a transfer from M to L. Note that the photons have different characteristic wavelengths.

In fact, on closer examination of the atom and its electron shells, it can be seen that the shells are divided into subshells as shown in Figure 1.5 below. For this reason, Kα radiation can be divided into $K\alpha_1$ and $K\alpha_2$ radiation, Kβ radiation into $K\beta_1$ and $K\beta_2$ radiation, and so on. The difference between the wavelengths of photons produced by the transfer of electrons of different subshells within the same shell is very small.

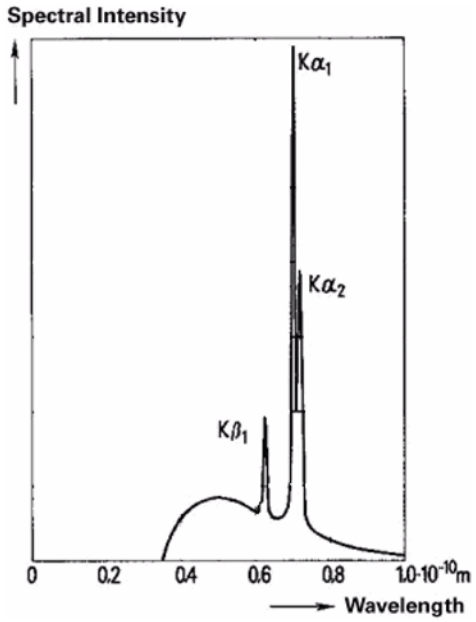
Figure 1.5 — Subshells and their transferred electrons



In Figure 1.6 below, the wavelength distribution of both continuous and characteristic radiation is shown as a function of intensity or the number of pulse counts per second. The characteristic peaks $K\alpha_1$, $K\alpha_2$, and $K\beta_1$ are clearly visible above the continuous spectrum.

The point on the wavelength scale at which the continuous spectrum begins is known as the short wavelength limit (SWL) and corresponds to the radiation produced by the electrons that give up all their energy on the initial impact. Thus for a particular supply voltage, these electrons give rise to photons of maximum energy (i.e., minimum wavelength). With an increase in supply voltage, the SWL as well as the point of maximum intensity of the continuous spectrum moves down the wavelength scale. In other words, an increase in operating potential produces a shift of the continuous spectrum in the direction of lower wavelengths and higher energy. On the other hand, the characteristic spectrum, because it is characteristic of the anode metal, merely undergoes an increase in intensity (i.e., pulse count rate).

Figure 1.6 — Spectrum of an X-ray tube



Biological Effects of X-Rays

Mechanisms of Damage

Injury to living tissue results from the transfer of energy to atoms and molecules in the cellular structure. Ionizing radiation causes atoms and molecules to become ionized or excited. These excitations and ionizations can:

- Produce free radicals;
- Break chemical bonds;
- Produce new chemical bonds and cross-linkage between macromolecules;
- Damage molecules that regulate vital cell processes (e.g. DNA, RNA, proteins).

The cell can repair certain levels of cell damage. At low doses (such as that received every day from background radiation), cellular damage is rapidly repaired.

At higher levels, cell death results. At extremely high doses, cells cannot be replaced quickly enough, and tissues fail to function.

Tissue Sensitivity

In general, the radiation sensitivity of a tissue is:

- proportional to the rate of proliferation of its cells;
- inversely proportional to the degree of cell differentiation.

For example, the following tissues and organs are listed from most-radiosensitive to least-radiosensitive:

1. Blood-forming organs
2. Reproductive organs
3. Skin
4. Bone and teeth
5. Muscle
6. Nervous system

This also means that a developing embryo is most sensitive to radiation during the early stages of differentiation, and an embryo/fetus is more sensitive to radiation exposure in the **first** trimester than in later trimesters.

Prompt and Delayed Effects

Radiation effects can be categorized by **when** they appear:

- **Prompt effects:** effects, including radiation sickness and radiation burns, seen immediately after large doses of radiation delivered over short periods of time.
- **Delayed effects:** effects such as cancer induction that may appear months or years after a radiation exposure

Delayed Effects of Radiation Exposure: Cancer

Studies of people exposed to high doses of radiation have shown that there is a risk of cancer induction associated with high doses.

- The specific types of cancers associated with radiation exposure include leukemia, multiple myeloma, breast cancer, lung cancer, and skin cancer.
- Radiation-induced cancers may take 10 - 15 years or more to appear.
- There **may** be a risk of cancer at low doses as well.

1.4.5 Beryllium Safety

DANGER

This product contains beryllium, a toxic metal used in the radiation outlet window of the X-ray optics. Fumes or dust from beryllium and its compounds can be hazardous if inhaled!

Beryllium must not be cut, machined, or handled under any circumstances.

Disposal of beryllium must comply with all applicable national, state, and local regulations.

1.4.6 Perchlorate Safety

The SMART X2S uses a lithium coin battery that contains perchlorate, a hazardous material.

Disposal of perchlorate must comply with all applicable national, state, and local regulations.

1.5 Help and Technical Support

1.5.1 Help within the Interface

Context-sensitive help is available by simply pressing the **Help** button on the touchscreen (Figure 1.7).

Figure 1.7 — Help button

1.5.2 Technical Support from Bruker Service Centers

You are invited to contact Bruker AXS whenever there are problems or questions related to the system. Before contacting Bruker AXS, please:

- Have the system's serial number available;
- Determine the system's software version (if you suspect a software problem);
- Record any error messages that appear; and
- Determine steps and conditions that recreate the problem (if possible).

CAUTION

Failure to refer instrument servicing to qualified Bruker personnel may result in injury or property damage!

North American Service Center Contact Information

Table 1.4 — Bruker AXS North American Service Center contact information

Bruker AXS North American Service Center	
Address:	Bruker AXS Inc. Customer Support 5465 East Cheryl Parkway Madison, WI 53711-5373 USA
Toll-free telephone:	1 (800) 234-XRAY [9729]
Direct line:	1 (608) 276-3000
Fax:	1 (608) 276-9162
E-mail:	Customer.Service@bruker-axs.com
Web:	http://www.bruker-axs.com

Karlsruhe Service Center Contact Information

Table 1.5 — Bruker AXS Karlsruhe Service Center contact information

Bruker AXS Karlsruhe Service Center	
Address:	Bruker AXS GmbH Customer Support Östliche Rheinbrückenstr. 49 76187 Karlsruhe Germany
Telephone:	+49 (721) 595-8403
XRD Hotline:	+49 (721) 50997 5208
E-mail:	service@bruker-axs.de
Web:	http://www.bruker-axs.de

2 Introduction to the SMART X2S

2.1 SMART X2S Features

The SMART X2S is designed specifically for walk-up structure solution for the working chemist.

Features of the SMART X2S include:

- Completely automated operation without user intervention—from sample loading and alignment through data collection and structure solution and refinement;
- Designed for the non-specialist. The automation software combines expert knowledge of structural chemistry with the power of cutting-edge data processing for structure solution and refinement at the level of research instrumentation at laboratories worldwide. The SMART X2S software automatically determines the structure of most routine organic and coordination compounds.
- Extremely compact, lightweight, and completely air-cooled;
- Requires only standard AC power to operate, drawing one-tenth the power of a standard diffractometer; and
- Closed-beam (i.e., the sample is inserted through an external port and then loaded and aligned automatically; users never need to put their hands into the enclosure).

For more information about the theory behind the SMART X2S, refer to Bruker AXS' Application Note A86-Exx003 Fundamentals of Single Crystal Diffraction.

Before using your SMART X2S, check that it is properly installed and in proper working order (e.g., that the touch-screen interface appears when the system is powered up).

2.2 Diagrams

Figure 2.1 — Front panel diagram

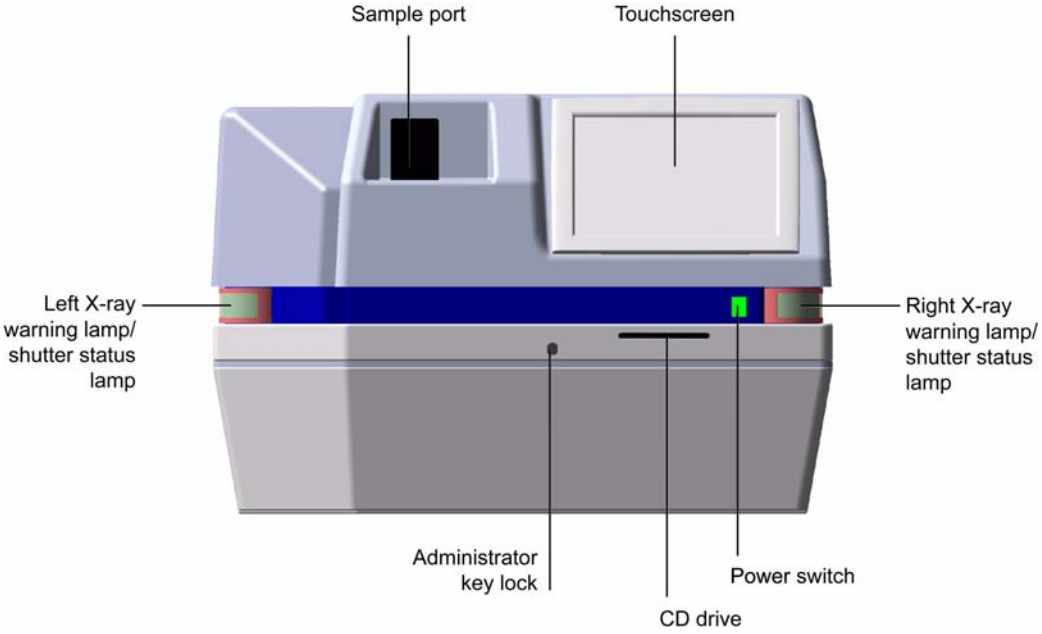
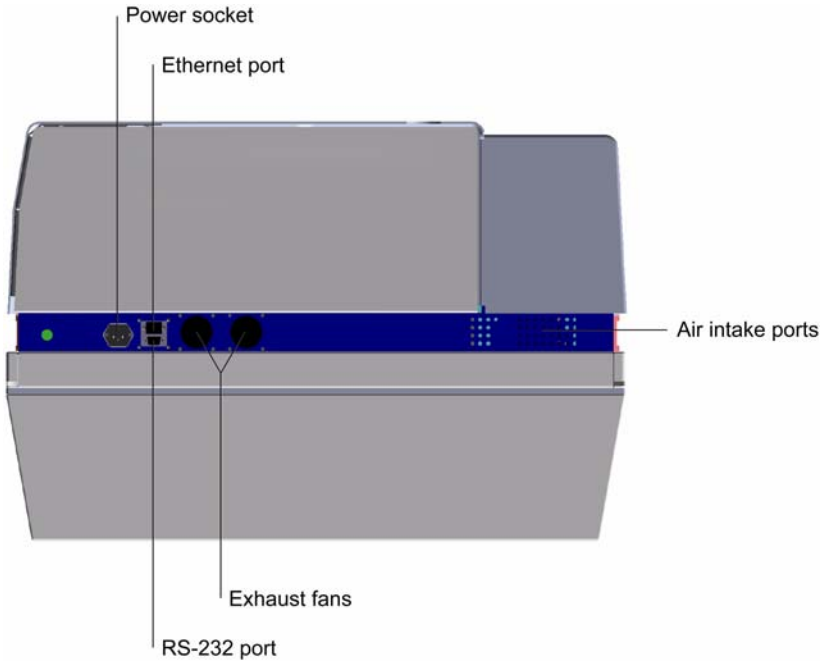


Figure 2.2 — Rear panel diagram



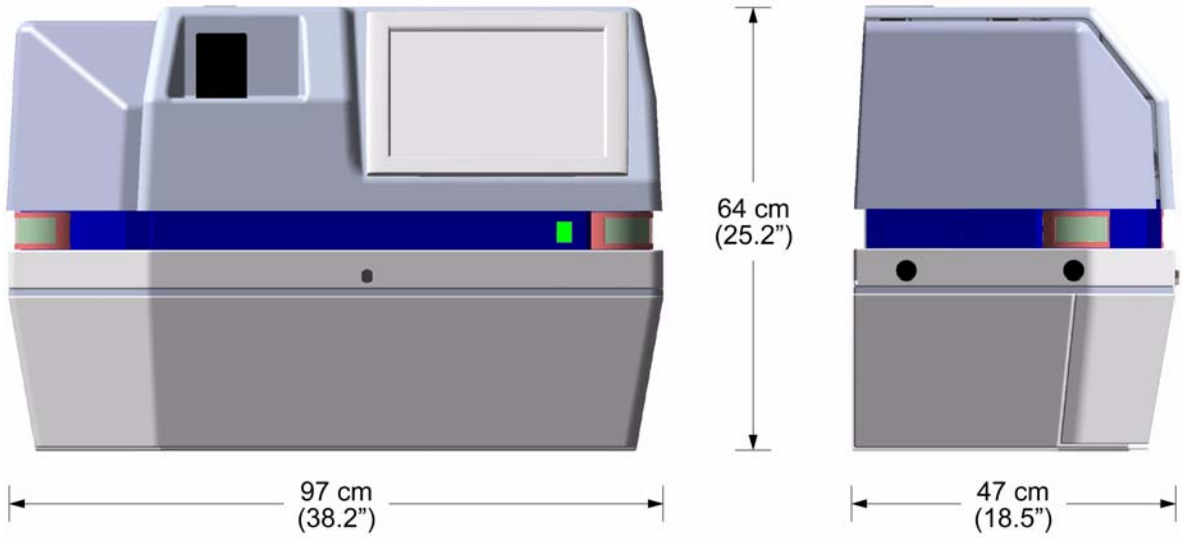
2.3 Technical Specifications

2.3.1 Dimensions and Weight

Table 2.1 — SMART X2S dimensions and weight

Height	Width	Depth	Weight
64 cm (25.2”)	97 cm (38.2”)	47 cm (18.5”)	150 kg (331 lbs)

Figure 2.3 — SMART X2S dimensions



2.3.2 Power Requirements

Table 2.2 — SMART X2S power requirements

Power Requirements	
Power:	110/220 VAC (± 10%), 50/60 Hz, 1-phase, 300W
Fuse:	Type 3.15, Time Lag, 250 V, 5×20 mm

CAUTION

It is important to be able to easily disconnect the SMART X2S from mains power in the event of an emergency or for service. Do not position the SMART X2S such that it is difficult to disconnect from the mains power supply.

2.3.3 Environment Requirements

Table 2.3 — SMART X2S environment requirements

Environment Requirements	
Installation surface	Horizontal tabletop, countertop, or other stable, vibration-free surface rated for the weight of the SMART X2S. For additional stability, the SMART X2S may be bolted to the installation surface.
Heat dissipation	less than 300 W (1024 btu/hr)
Clearance behind	at least 3” (7.6 cm) for proper airflow and ventilation
Clearance above	at least 3’ (.91 m) for service access
Altitude	up to 6562’ (2000 m) above sea level
Ambient temperature range	59-77°F (15-25°C)
Ambient humidity range	20%-80%, non-condensing

NOTE: The SMART X2S is designed for indoor use only.

2.3.4 Other Specifications

Table 2.4 — SMART X2S other specifications

Specification	Value
SMART X2S Electronic Components Overvoltage Category	II
SMART X2S Pollution Degree	2
X-ray Tube	50 W microfocus tube, molybdenum anode, air-cooled
X-ray Optics	Toroidally-curved Si crystals for three-dimensionally-focused, monochromatic X-rays with very high flux density
CCD Detector	Air-cooled, no spatial distortion
Sample Mount Type	Bruker Spine Pin
Low-temperature Device (optional)	Supports DTC (Desktop Cooler) low-temperature device
Data Collection Resolution	To IUCr standards

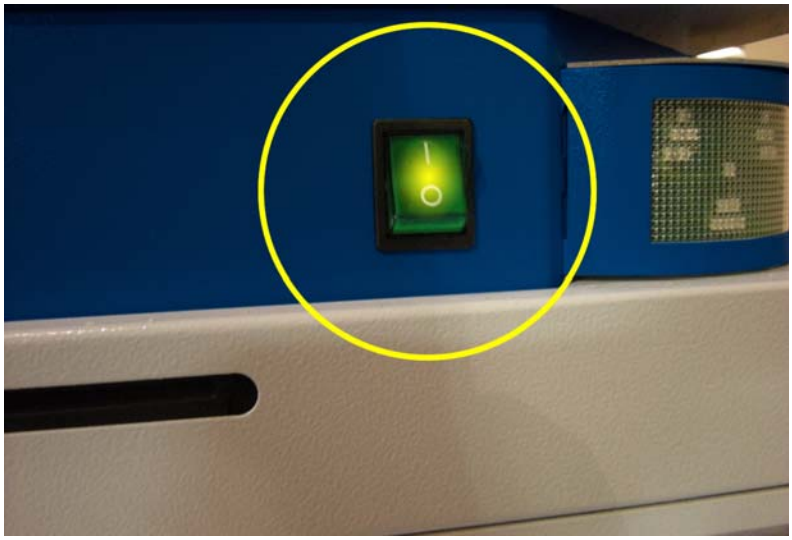
2.4 Startup and Shutdown

2.4.1 Starting Up the SMART X2S

1. Some SMART X2S units have a safety key switch that must be unlocked before the system can be turned on. If you have a safety key switch, turn it to the “On” position.
2. Press the power switch on the front panel to the “On” position.

   The power switch illuminates.

Figure 2.4 — Power switch



The system beeps and the touchscreen displays the system BIOS (during the CPU’s self-test).

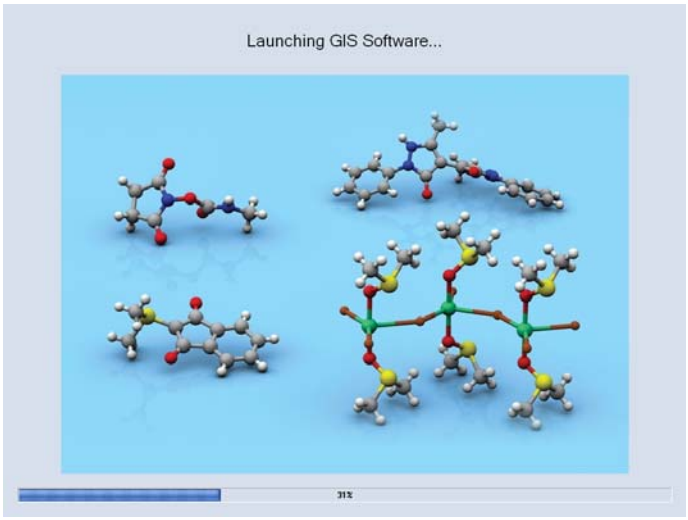
After about one more minute, the SMART X2S begins to initialize.

First, the instrument initializes its serial ports.

Figure 2.5 — Initializing serial ports

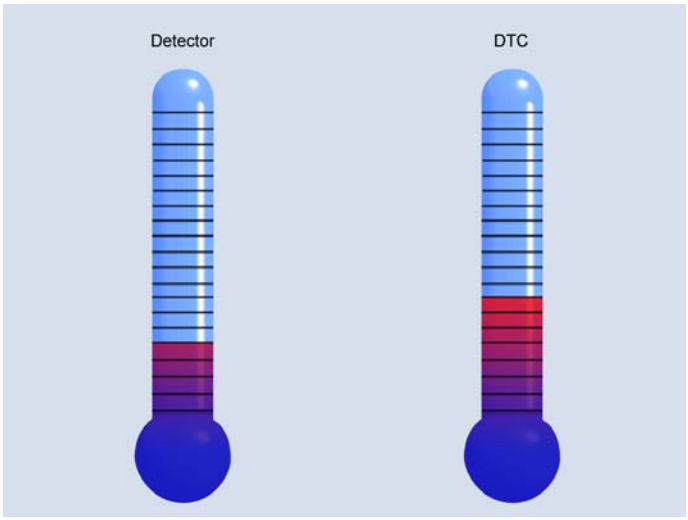
Then, the instrument starts GIS, the control software for the SMART X2S hardware.

Figure 2.6 — Starting GIS



After the system finishes initializing, it begins cooling the detector and desktop cooler (if present). As cooling proceeds, the system displays the temperatures graphically.

Figure 2.7 — Cooling displays



After cooling is complete, the kiosk-style interface appears.

Figure 2.8 — Starting kiosk application

Finally, the system checks whether a sample is loaded. If a sample is loaded, the instrument will eject the sample and make it available at the sample port. If no sample is loaded, the instrument will display the “Welcome” screen.

Figure 2.9 — Kiosk “Welcome” screen

2.4.2 Shutting Down the SMART X2S

1. Flip the power switch on the front of the SMART X2S to the “Off” position (“0”).
2. If your SMART X2S unit has a safety key switch, turn it to the “Off” position and remove it to prevent unauthorized access.

3 Sample Preparation and Mounting

To study a sample with the SMART X2S, the sample must be mounted on a Bruker Spine Pin.

3.1 Sample Preparation Overview

The process of sample mounting is simple: from the many crystals within a bulk sample, identify the best candidate for study and affix it to the Bruker Spine Pin with a special ultraviolet-curable adhesive. Once the adhesive is cured, the sample is ready for use with the SMART X2S.

You will need:

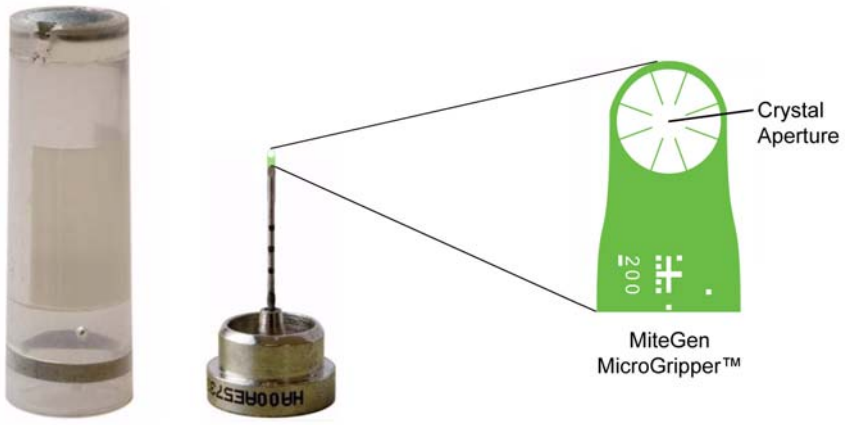
- Your bulk sample;
- A microscope for identifying suitable candidate crystals for study;
- A preparation needle or other tool for separating the candidate crystals;
- A Bruker Spine Pin micromount and cap;
- Ultraviolet-curable adhesive to fix the crystal on the Bruker Spine Pin; and
- An ultraviolet penlight for rapidly curing the adhesive.

3.2 The Bruker Spine Pin

The Bruker Spine Pin uses a MiTeGen MicroGripper™, precision-manufactured to work properly within the SMART X2S. The Pin has a magnetic cap that protects the sample.

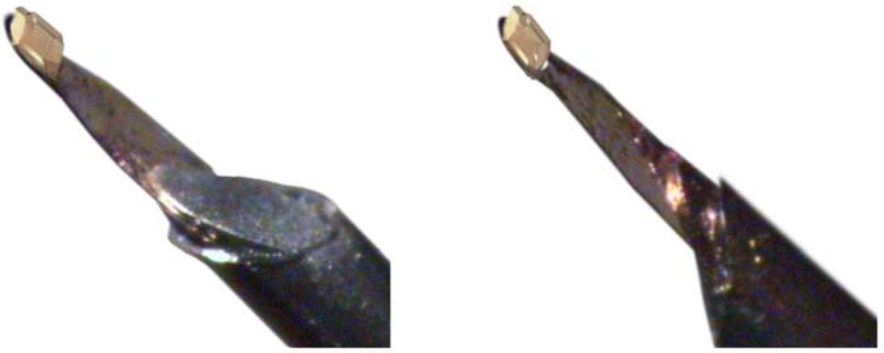
The crystal needs to be attached across the crystal aperture at the tip of the MicroGripper™.

Figure 3.1 — Bruker Spine Pin with cap, crystal aperture at tip of MicroGripper™



NOTE: When attaching the crystal, be sure to attach it to the inner surface of the MicroGripper™ (Figure 3.2). The inner surface will be readily visible under the microscope.

Figure 3.2 — Proper crystal mounting


Inner Surface (Correct)
When the crystal is in the crystal aperture and on the inner surface of the MicroGripper™, the SMART X2S will align the crystal precisely to the center of the instrument. The aperture size will be readable.
Outer Surface (Incorrect)
If the crystal is positioned on the outer surface of the MicroGripper™, the SMART X2S will be unable to position the crystal. The aperture size will appear backwards.

3.2.1 Reusing Bruker Spine Pins

Bruker Spine pins may be reused. The ultraviolet-curable glue dissolves in hot water.

3.3 Sample Preparation Procedure

3.3.1 Identifying Suitable Crystals

Begin by using the microscope to look for a suitable crystal in the bulk sample. The ideal crystal should be:

- Uniform in color;
- Free of cracks and inclusions;
- Without attached crystallites; and
- isometric (i.e., the same dimensions in all directions). The ideal crystal is about 0.5 mm in all directions.

Figure 3.3 — Bulk crystals on microscope slide

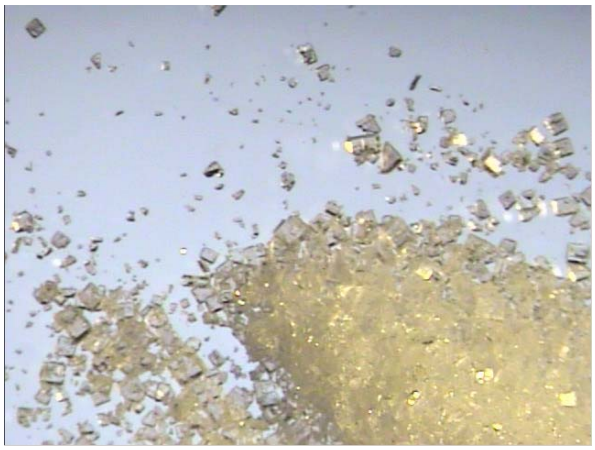
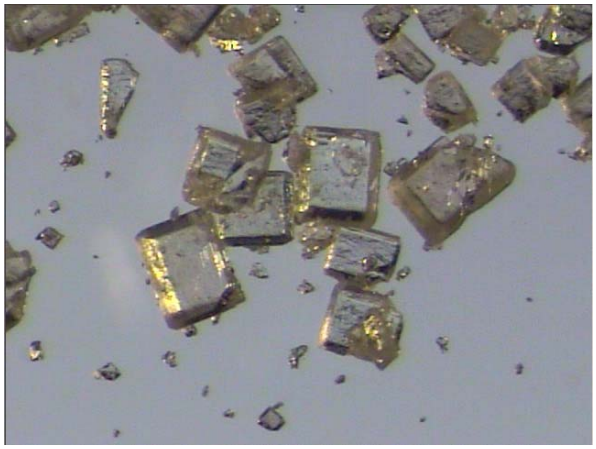


Figure 3.4 — Strong candidates for study



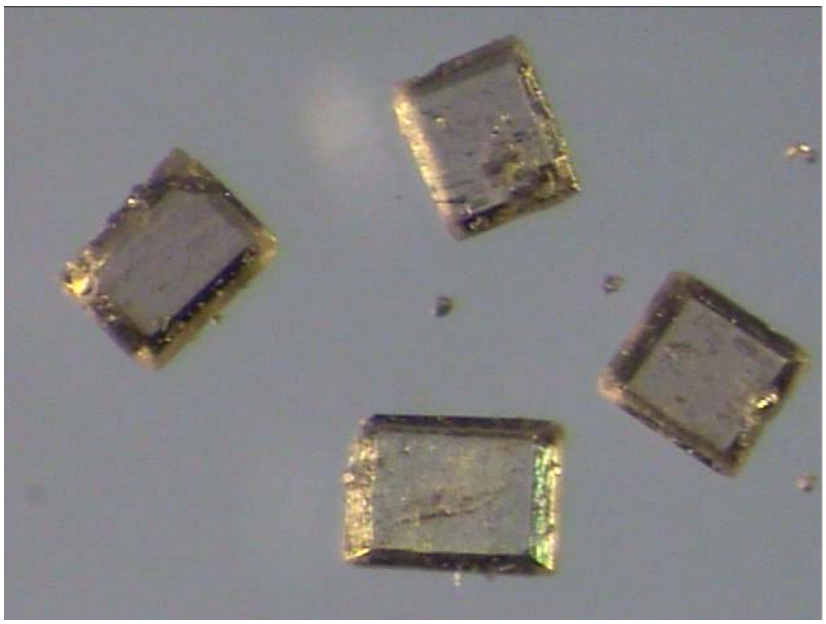
Problems Mounting Certain Crystals

NOTE: Some water-soluble crystals may not work with the ultraviolet-curable adhesive. Super Glue® may be used in such cases.

3.3.2 Separating the Crystals

1. Isolate suitable crystals from the bulk sample, and move them to a separate area on the microscope slide. Compare the crystals, and choose the best one.

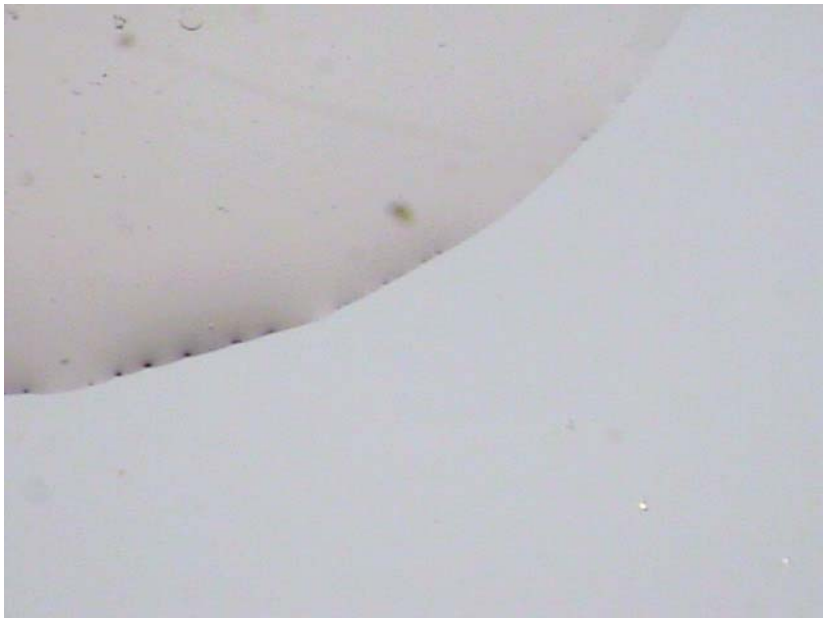
Figure 3.5 — Candidate crystals, separated from bulk sample



3.3.3 Wetting the Micromount with Adhesive

1. Add a drop of adhesive to the microscope slide, away from the chosen crystals. We will use this drop to wet the aperture of the micromount.

Figure 3.6 — Adhesive on the microscope slide



NOTE: The adhesive can be used to “wash” crystallites from the surface of the candidate crystal. Be careful that the flowing adhesive does not carry the crystal out of the microscope’s field of view.

2. Dip the aperture of the MicroGripper™ into the adhesive to wet it.

Figure 3.7 — MicroGripper™

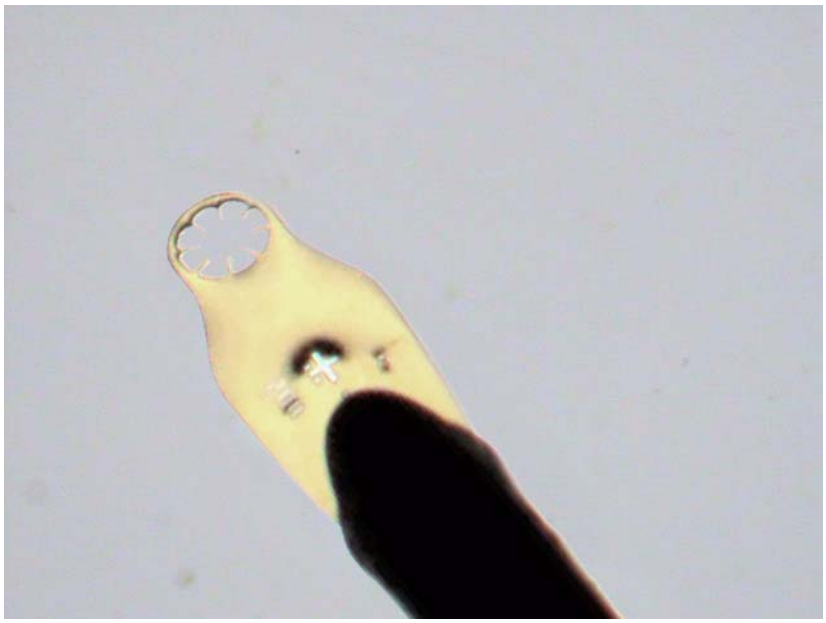
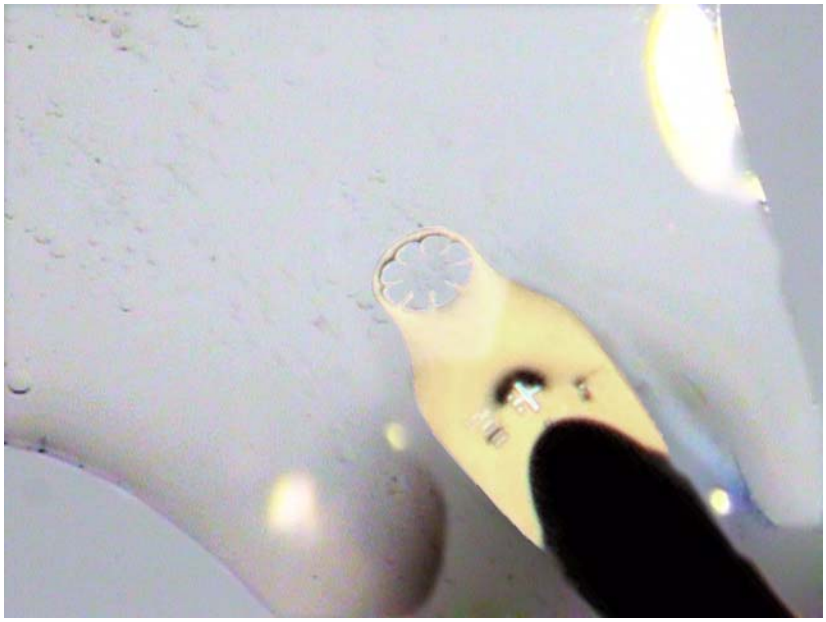


Figure 3.8 — MicroGripper™ aperture in adhesive



3.3.4 Attaching the Crystal to the MicroGripper™

1. Scoop up the desired crystal so that it is in the center of the MicroGripper™ aperture.

NOTE: Make sure that the crystal is in the aperture. If the crystal is not in the aperture, the SMART X2S may not be able to collect data.

Figure 3.9 — MicroGripper™ near desired crystal

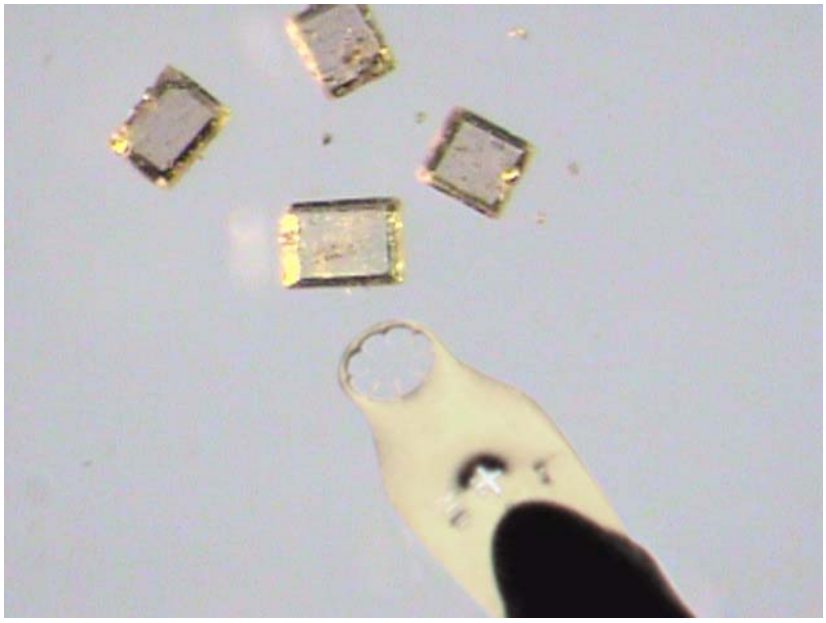
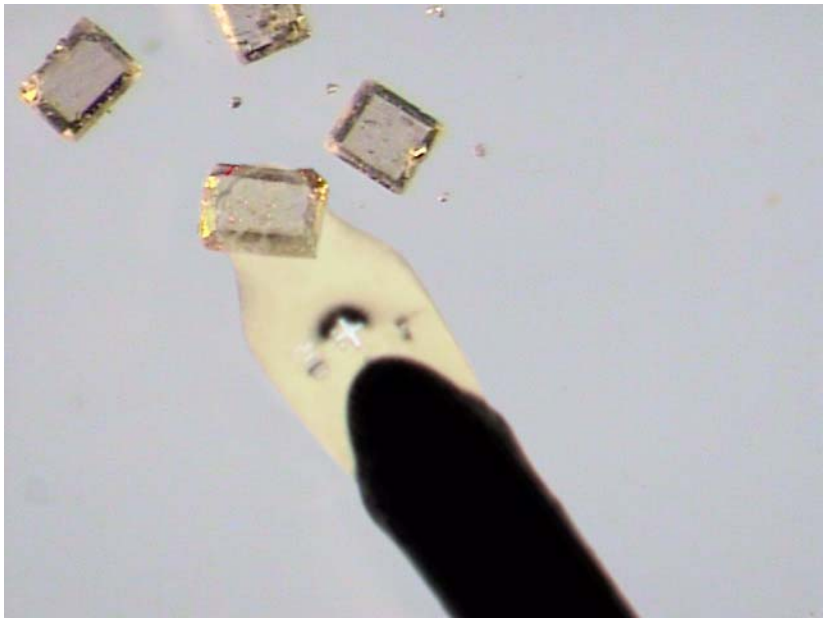


Figure 3.10 —Crystal in MicroGripper™ aperture



3.3.5 Curing the Adhesive with Ultraviolet Light

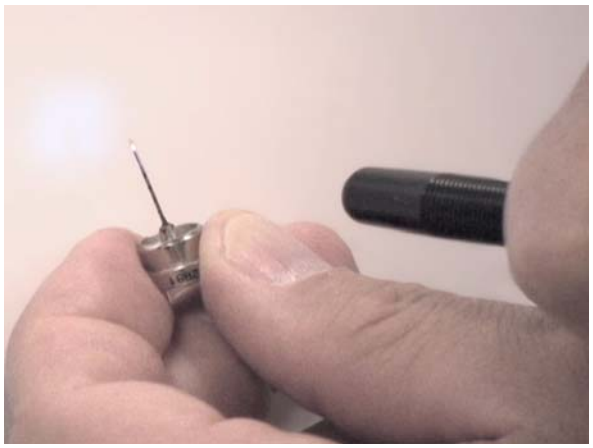
Ultraviolet-curable adhesive leaves ample time for the crystal to be manipulated. When the crystal is in the proper place, it may be fixed within seconds by shining ultraviolet light on it.

CAUTION

The ultraviolet pen light radiates intense ultraviolet light when the button is pressed. Do not look directly into the ultraviolet light during operation of the pen light. Exposure to intense UV light, even for a brief period, can harm the eyes. If viewing the UV light is necessary, use UV-filtered glasses to avoid eye damage. Keep the ultraviolet pen light out of the reach of children. Avoid direct exposure to ultraviolet light.

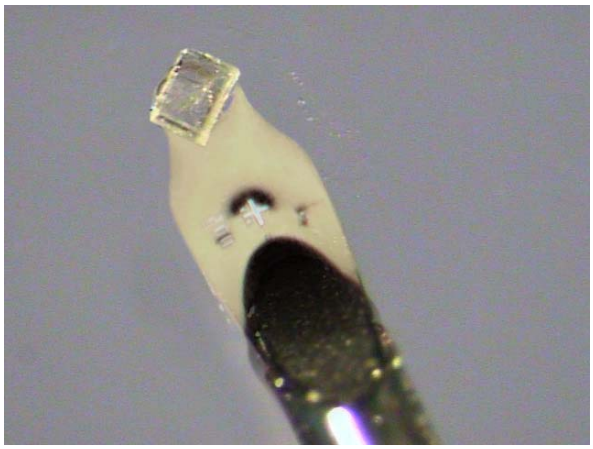
1. When you have the desired crystal in the center of the micromount's aperture, cure the adhesive by shining the ultraviolet pen light on the sample for about 20 seconds.

Figure 3.11 —Adhesive illuminated by ultraviolet pen light



2. When the adhesive is cured, place the Bruker Spine Pin in its protective cap. The sample is now ready for use with the SMART X2S.

Figure 3.12 —Successfully mounted crystal



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4 Setting Up Data Collection

4.1 The SMART X2S Touchscreen Interface

The SMART X2S features an intuitive, kiosk-style interface with input through a touchscreen. The interface guides the user through the experiment, providing easy-to-understand graphical feedback about the status and quality of the structure determination process.

4.1.1 Main Buttons

Table 4.1 — SMART X2S main buttons

Button	Function
	Forward —Proceed to the next screen.
	Back — Ignore any data entered on the current screen, and return to the previous screen.
	Back to beginning — Ignore all data entered, and return to the Welcome Screen.
	Forward to CD burning — Proceed to the CD burning phase, skipping all steps in between.
	Help — Press at any time for context-sensitive help.
	Stop — Stop the instrument. When pressed, you are prompted to confirm. When you confirm, all internal movement stops and the experiment is aborted.
	Discard report — Throw away the report generated from the current dataset and return to the “Welcome” screen.

4.2 The “Welcome” Screen

The system displays a “Welcome” screen.

Touch the “Welcome” screen anywhere to begin.

Figure 4.1 — Welcome to the SMART X2S

4.3 Inserting an Empty CD

After touching the “Welcome” screen, the “Please insert an empty CD” screen appears.

Figure 4.2 — Please insert an empty CD

1. Insert an empty CD, label side up, into the slot on the front of the SMART X2S.

NOTE: The SMART X2S has no known issues with any CD-R media types.

Figure 4.3 — Inserting a CD

After the SMART X2S recognizes that an empty CD has been inserted, a confirmation screen will appear.

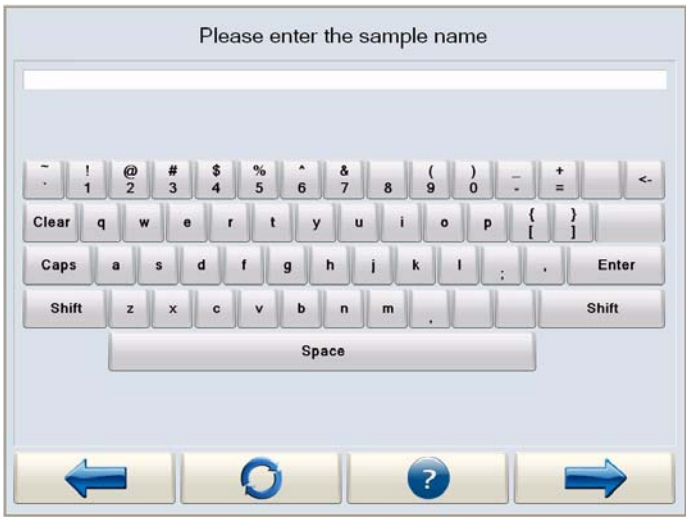
Figure 4.4 — Confirmation screen

The SMART X2S automatically proceeds to the “Please name your compound” screen.

4.4 Naming Your Sample

After inserting a blank CD, the “Please enter the sample name” screen appears.

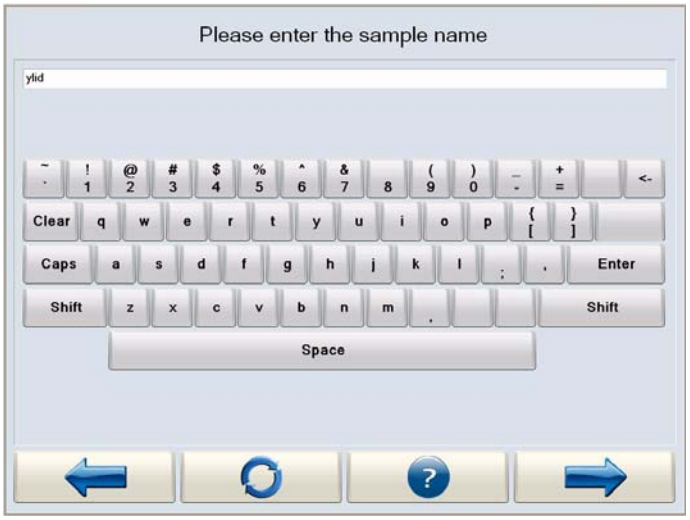
Figure 4.5 — Please enter the sample name



1. Use the keyboard on the touchscreen to name the compound. This is the name that will be used in the report generated by the SMART X2S.

NOTE: The compound name is limited to a maximum of 12 characters.

Figure 4.6 — Please enter the sample name (filled in)

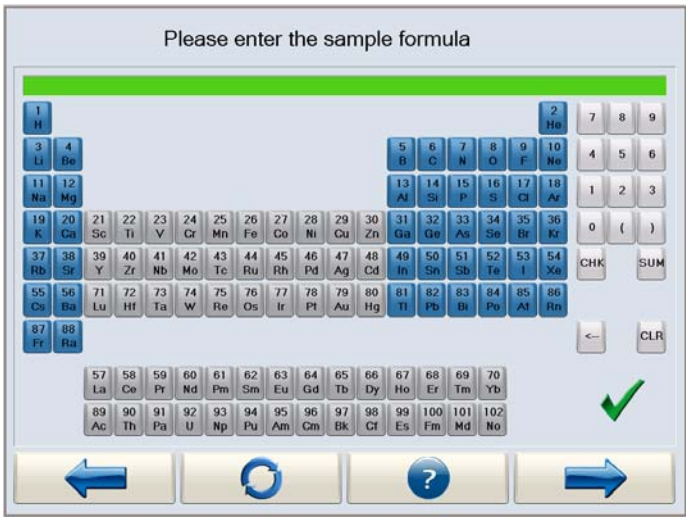


2. Press the **Forward** button , or [Enter] on the touchscreen, to proceed to the next screen.

4.5 Entering the Sample Formula

After naming the compound, the “Please enter the sample formula” screen appears.

Figure 4.7 — Please enter the sample formula

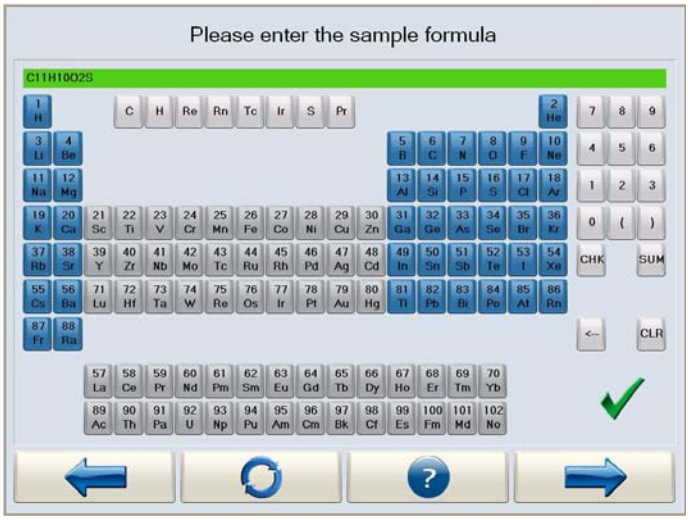


1. Use the periodic table’s element buttons to enter the sample formula.

NOTE: The **CHK** button checks the formula for consistency, and the **SUM** button sums up separate elements in the entry (e.g., `C4H4C4H4` becomes `C8H8` after pressing **SUM**).

NOTE: The number of atoms can be entered by repeatedly pressing the same key or by using the number pad.

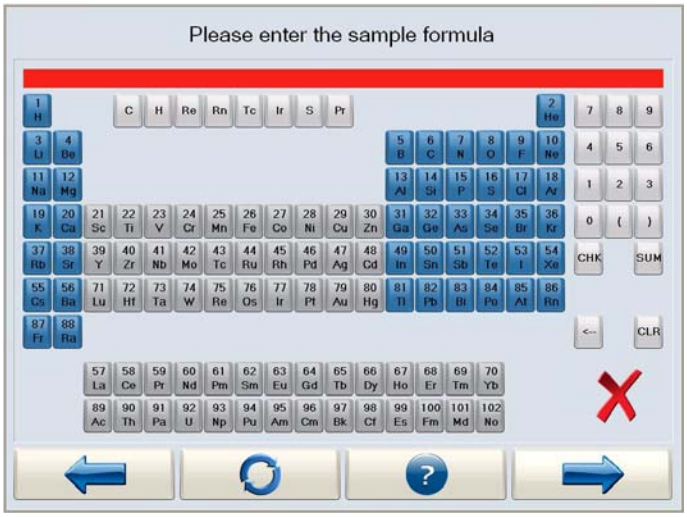
Figure 4.8 — Please enter the sample formula (filled in)



NOTE: The SMART X2S will learn the 8 most frequently-used elements and display them in a bar along the top of the periodic table.

If the formula is present and valid, a green check mark will appear in the lower right-hand corner of the screen. If the formula is not present or valid, this area will display a red “X”.

Figure 4.9 — Please enter the sample formula (red “X”)

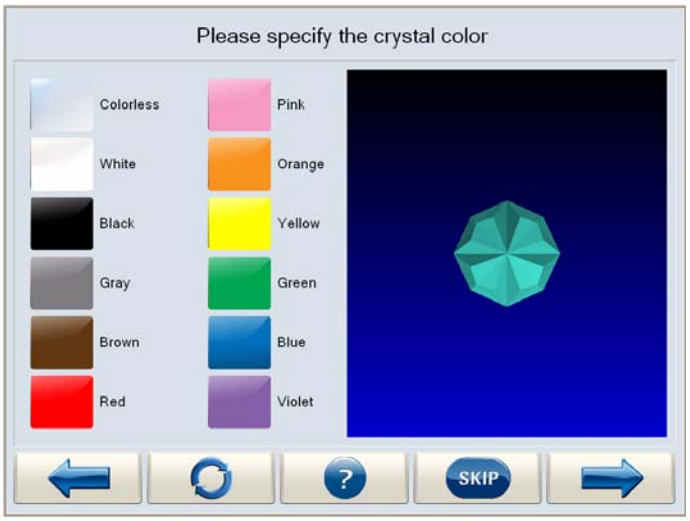


2. Press the **Forward** button to proceed to the next screen.

4.6 Specifying the Crystal Color

After entering the sample formula, the “Please specify the crystal color” screen appears (the color will be used in the report generated by the SMART X2S).

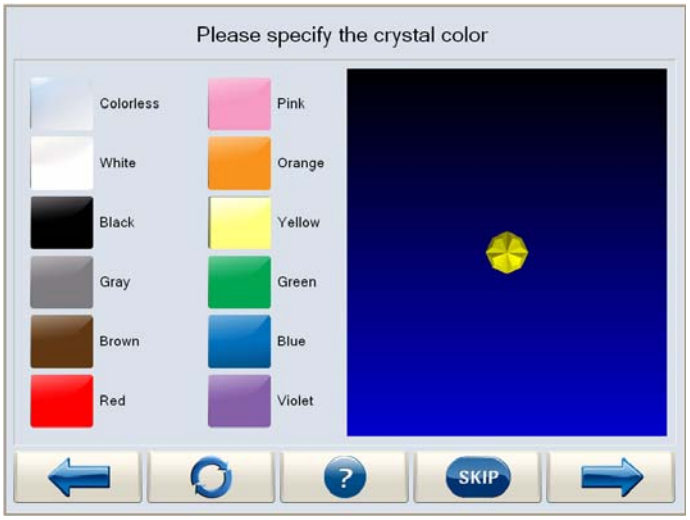
Figure 4.10 —Please specify the crystal color



1. Simply press the appropriate button on the touchscreen to choose the color.

NOTE: If desired, the color input can be skipped by pressing the **SKIP** button.

Figure 4.11 —Please specify the crystal color (yellow)

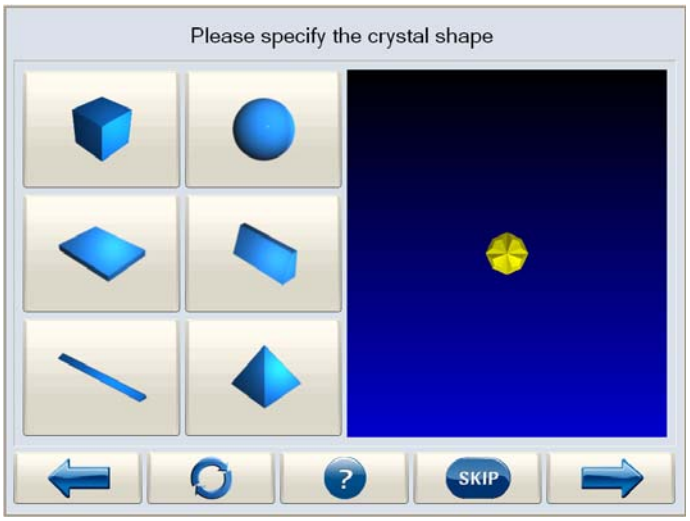


2. Press the **Forward** button to proceed to the next screen.

4.7 Specifying the Crystal Shape

After specifying the crystal color, the “Please specify the crystal shape” screen appears.

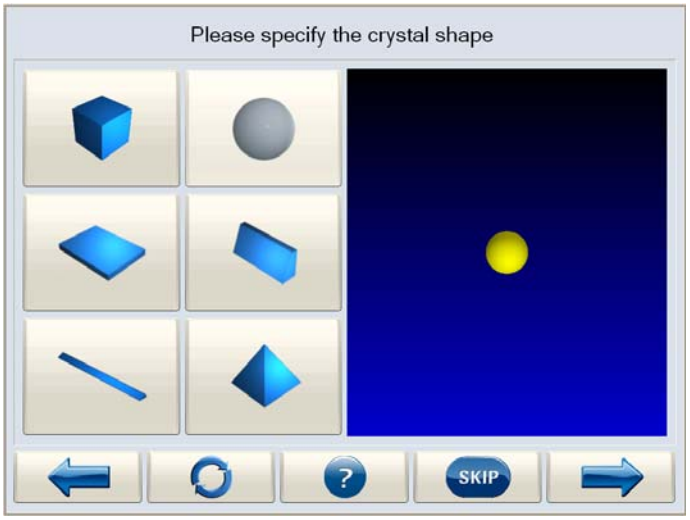
Figure 4.12 —Please specify the crystal shape



1. Choose the appropriate shape by pressing one of the shape buttons.

NOTE: If the shape is not necessary, press the **SKIP** button at the bottom of the screen.

Figure 4.13 —Please specify the crystal shape (sphere)

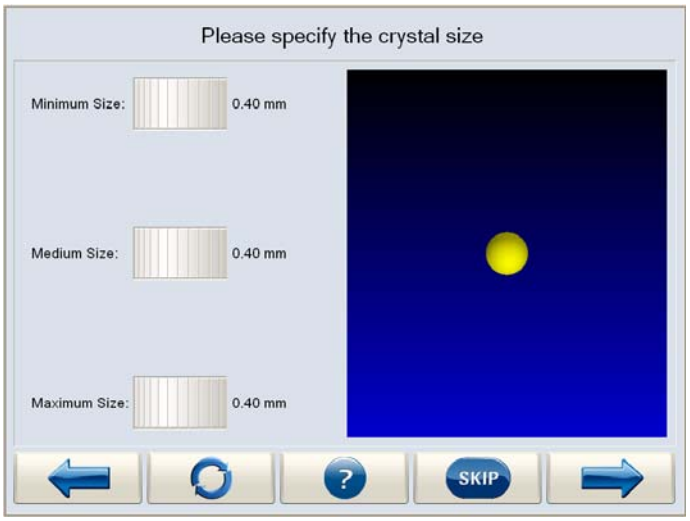


2. Press the **Forward** button to proceed to the next screen.

4.8 Specifying the Crystal Size

After specifying the crystal shape, the “Please specify the crystal size” screen appears.

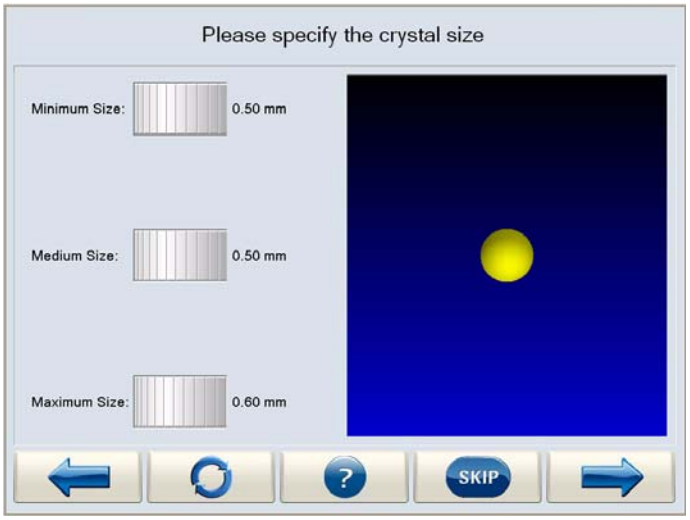
Figure 4.14 —Please specify the crystal size



1. Use the touchscreen controls to set the dimensions of the crystal.

NOTE: If the size is not known or not necessary, press the **SKIP** button at the bottom of the screen.

Figure 4.15 —Please choose your crystal’s size (0.50 mm × 0.50 mm × 0.60 mm chosen)



2. Press the **Forward** button to proceed to the next screen.

4.9 Selecting the Redundancy Mode

After specifying the crystal size, the “Please select the redundancy mode” screen appears.

Figure 4.16 —Please select the redundancy mode

1. Use the touchscreen controls to select the redundancy mode for the data collection:
   - The button on the left (activated by default) chooses standard redundancy mode (3 data collections).
   - The button on the right chooses extended redundancy mode (6 data collections).

NOTE: When extended redundancy mode is used, the data collection time will be approximately twice as long as in standard redundancy mode.

2. Press the **Forward** button to proceed to the next screen.

4.10 Inserting the Sample

After specifying the crystal size, the SMART X2S prompts for the sample.

Figure 4.17 —Please insert your sample to begin processing

1. Insert the sample vial into the sample port on the front of the SMART X2S.

NOTE: Leave the protective cap on the sample when inserting it.

Figure 4.18 —Inserting the sample

The sample loader mechanism automatically moves the sample into the SMART X2S.

After inserting the sample, the SMART X2S automatically aligns it and begins collecting data.

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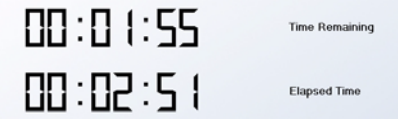
5 Data Collection and Structure Solution

5.1 The “Processing” Screen

5.1.1 Time Displays

The Time Displays give at-a-glance information about the data collection process. Time Remaining and Elapsed Time are presented.

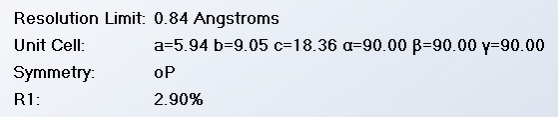
Figure 5.1 — Time Displays



5.1.2 Crystal Information

Below the Process Steps and Time Displays are the Crystal Information area, which gives at-a-glance information about the crystal: Resolution Limit, Unit Cell parameters, Symmetry, and R1. These readouts update as data is collected.

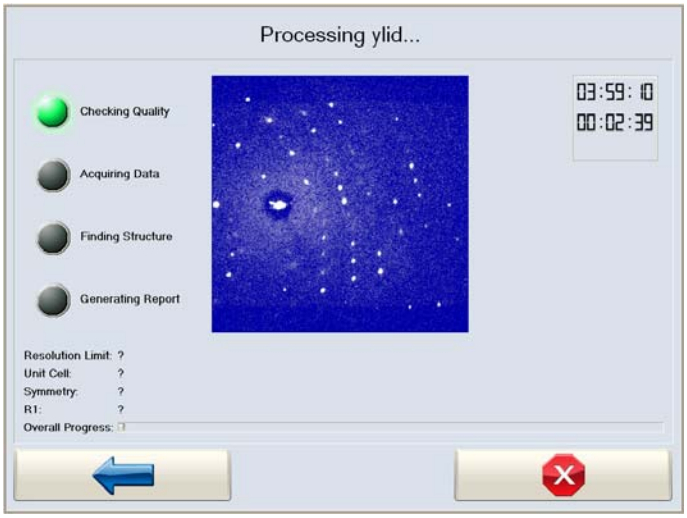
Figure 5.2 — Crystal Information area



5.1.3 Detector Frame Display

While collecting data, the SMART X2S displays the current detector frame in the upper right-hand corner of the screen. Touch the frame to exchange the positions of the Detector Frame and Time Displays, providing a larger view. To return to the original view, simply touch the Time Displays.

Figure 5.3 — Detector frame display



5.1.4 Process Steps

To the left of the Time Displays are the Process Steps:

- Checking Quality;
- Acquiring Data;
- Finding Structure; and
- Generating Report.

As the SMART X2S proceeds through the experiment, it moves sequentially through these steps.

Each step has a status icon (Table 5.1) that shows the SMART X2S level of success in performing that step.

Table 5.1 — Process steps: status icons

Icon	Description
	Successful.
	Successful, but there may be a problem with data.
	Unsuccessful; unable to perform step.
	Step complete.
	Step not attempted yet.

Checking Quality

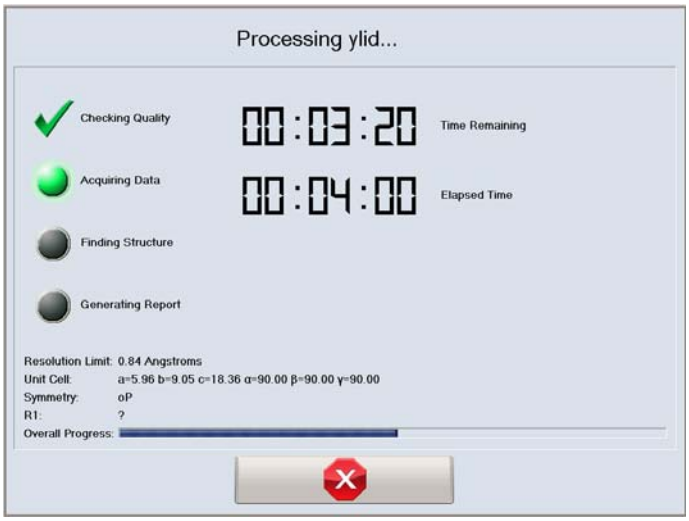
The SMART X2S begins by collecting data to determine the orientation matrix and evaluating the mosaicity of the crystal.

Figure 5.4 — Checking quality

Acquiring Data

After indexing the unit cell and finding a suitable maximum resolution, data collection begins. The SMART X2S integrates the data, scales it, and determines the Laue class during data acquisition.

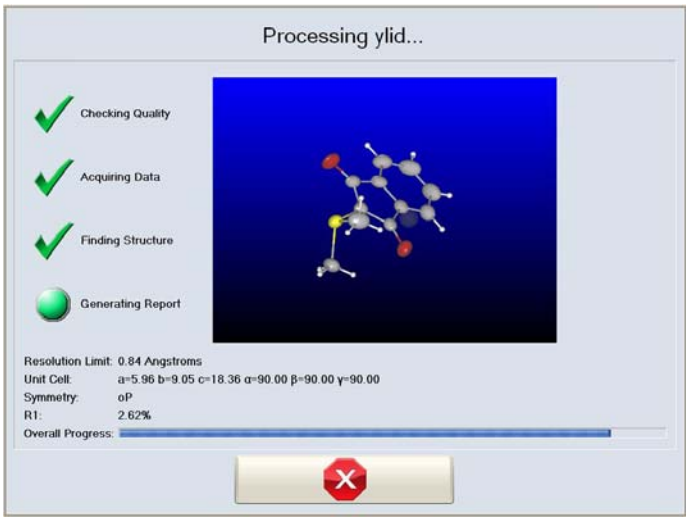
Figure 5.5 — Acquiring data



Finding Structure

After data collection is complete, the SMART X2S solves the structure. The structure solution software moves through Patterson, direct, and dual-space methods to ensure that the structure is correctly solved. Atoms are assigned using rigorous geometry checks and rigid-bond tests of thermal parameters. The results are then verified against International Union of Crystallography standards.

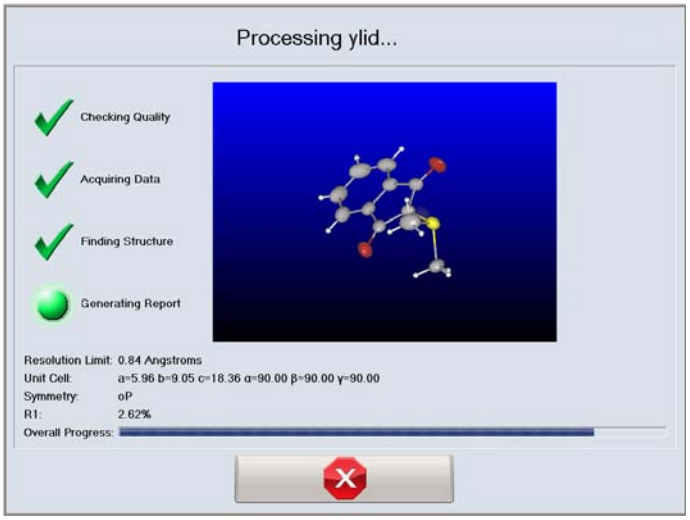
Figure 5.6 — Finding structure



Generating Report

After the structure determination, the SMART X2S generates the report that will appear on the CD. The report can be previewed prior to burning the CD.

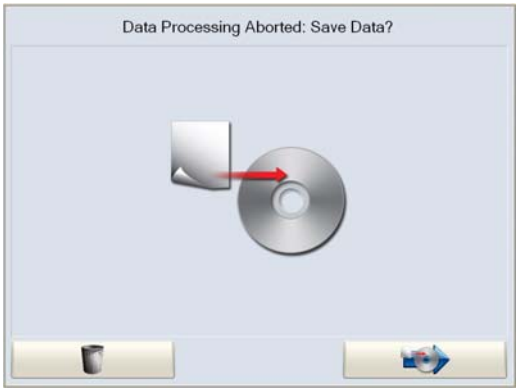
Figure 5.7 — Generating report



5.2 Aborting Data Processing

If you touch the button while collecting or processing data, the SMART X2S will stop. After the system has stopped, choose whether to delete the collected data, or write it to the CD.

Figure 5.8 — “Data Processing Aborted” screen



If you choose to delete the collected data, the system deletes the data and returns to the “Welcome” screen.

To write the data to the CD, press the button. The system then proceeds to the “CD Writing”screen.

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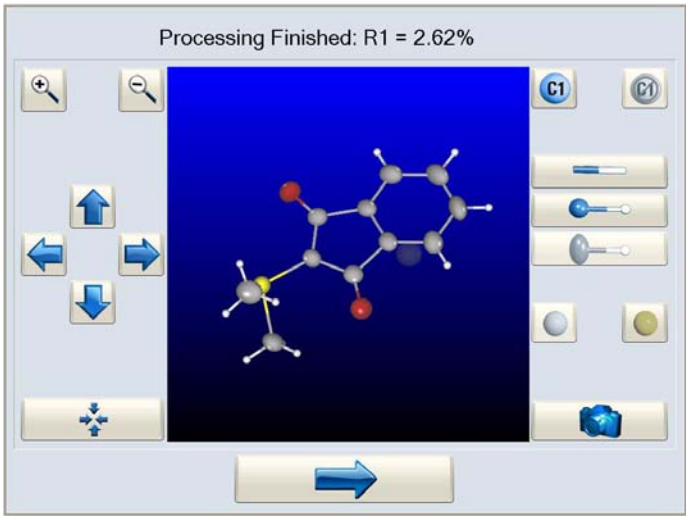
6 Structure View, Report Display, and CD Burning

6.1 Structure View

After refining the structure and generating the report, the SMART X2S displays the structure in a 3D view that can be manipulated by simply touching the touchscreen.

The structure appears in standard CPK colors.

Figure 6.1 — Structure view



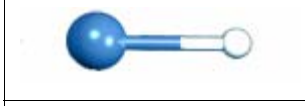
To view the report, press the **Forward** button to proceed to the report screen.

6.1.1 Structure View Button Functions

Table 6.1 — Structure View button functions (left side)

Button	Function
	Zoom in — Zoom into display less of the structure.
	Zoom out — Zoom out to display more of the structure.
	Translate up — Move the structure up.
	Translate left — Move the structure left.
	Translate right — Move the structure right.
	Translate down — Move the structure down.
	Reset view — Undo all translations, rotations, and zooms. Return the structure to the initial view.

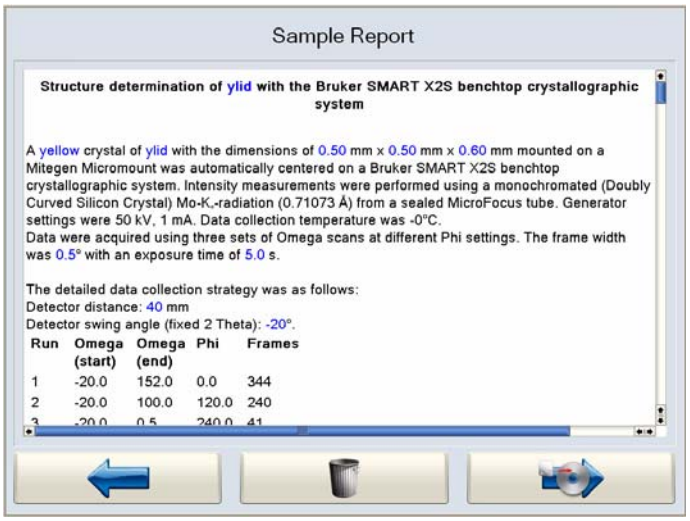
Table 6.2 — Structure View button functions (right side)

Button	Function
	Atom labels visible — Turn atom labels on.
	Atom labels hidden — Turn atom labels off.
	Pipes display — Display the structure as pipes.
	**Ball-and-stick display** — Display the structure as a ball-and-stick model.
	Thermal ellipsoid display — Display the structure with ellipsoids representing atomic motion.
	Residual peak visible — Show the strongest residual electron density peak (i.e., unassigned peak). The strength of the Q peak is represented by the sphere's opacity.
	Residual peak hidden — Hide the strongest residual peak.
	Snapshot — Save the current view of the structure as a .jpg file, which will be written to the CD when it is burned.

6.2 Report Display

After the “Structure View” screen, the SMART X2S displays the report that will be burned to the CD.

Figure 6.2 — Report display


Sample Report
Structure determination of ylid with the Bruker SMART X2S benchtop crystallographic system
A yellow crystal of ylid with the dimensions of 0.50 mm x 0.50 mm x 0.60 mm mounted on a Mitegen Micromount was automatically centered on a Bruker SMART X2S benchtop crystallographic system. Intensity measurements were performed using a monochromated (Doubly Curved Silicon Crystal) Mo-K,-radiation (0.71073 Å) from a sealed MicroFocus tube. Generator settings were 50 kV, 1 mA. Data collection temperature was -0°C.
Data were acquired using three sets of Omega scans at different Phi settings. The frame width was 0.5° with an exposure time of 5.0 s.
The detailed data collection strategy was as follows:
Detector distance: 40 mm
Detector swing angle (fixed 2 Theta): -20°.
Run Omega (start) Omega (end) Phi Frames
1 -20.0 152.0 0.0 344
2 -20.0 100.0 120.0 240

After examining the report:

- Press the button to go back to the “Structure View” screen;
- Press the button to discard the contents of the report; or
- Press the button to accept the report’s contents and burn them to the CD.

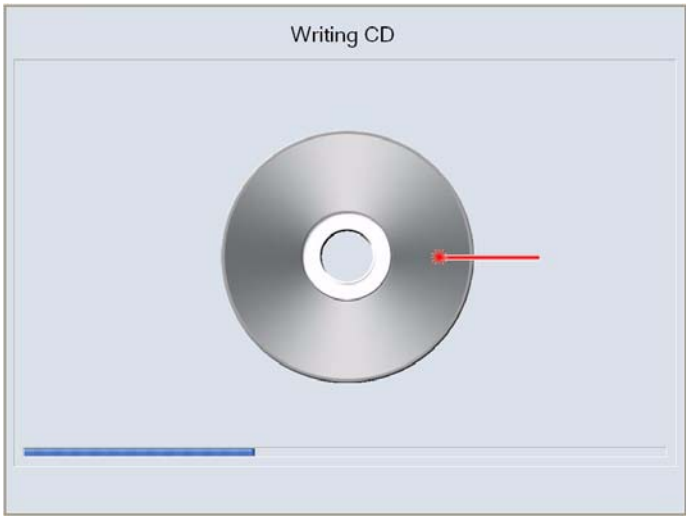
After pressing the button to discard the contents of the report, the system will prompt to confirm the decision. Press to go back, or to delete the report and return to the previous screen.

Figure 6.3 — Are you sure that you want to discard your results?

6.3 CD Burning

After accepting the contents of the report and pressing the button, the SMART X2S will burn the report, along with all data collected, onto the CD.

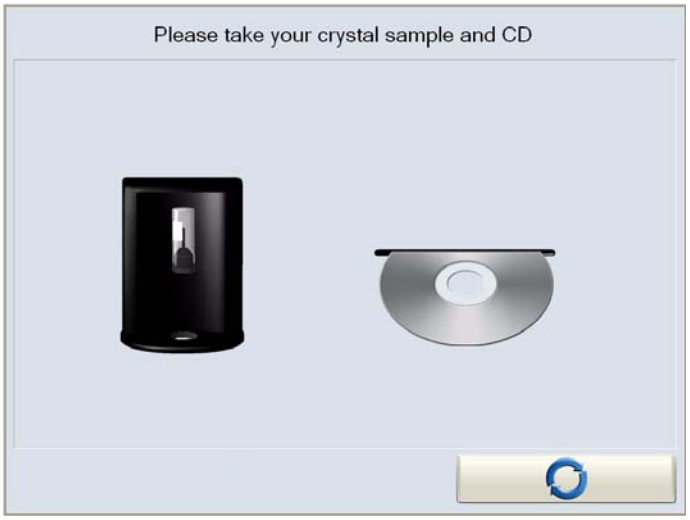
Figure 6.4 — Burning the CD



6.4 Removing the CD and Sample

When CD burning is complete, the SMART X2S will eject the CD. The sample will also appear at the sample port on the front of the SMART X2S. A screen appears prompting to remove the CD and sample.

Figure 6.5 — Please take your CD and sample



1. Remove the CD from the drive, and label it.
2. Remove the sample from the SMART X2S sample port.
3. Press the button to return to the “Welcome” screen.

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7 The Data CD

7.1 The Crystallographic Report

When the data CD is inserted into a computer with a CD-ROM drive, the crystallographic report automatically opens in your default web browser. The report contains four sections:

- Report Summary
- Molecule Viewer
- Detailed Report
- Alerts

7.1.1 Report Summary Section

The Report Summary gives information about the experiment and its results. Information includes:

- Crystal information (color, name, dimensions, mounting method);
- Radiation information (monochromatization method, wavelength, generator power);
- Experiment parameters (temperature, scan parameters, detector distance and swing angle);
- Unit cell parameters, space group, and Z-value;
- Structure parameters and results (integration, absorption correction, least squares, and electron density); and
- Version information for the various software modules used inside the SMART X2S.

Figure 7.1 — Report summary section

Structure determination of ylid with the Bruker SMART X2S benchtop crystallographic system

A yellow crystal of ylid with the dimensions of 0.50 mm x 0.50 mm x 0.60 mm mounted on a Mitegen Micromount was automatically centered on a Bruker SMART X2S benchtop crystallographic system. Intensity measurements were performed using a monochromated (Doubly Curved Silicon Crystal) Mo-K_α-radiation (0.71073 Å) from a sealed MicroFocus tube. Generator settings were 50 kV, 1 mA. Data collection temperature was 27°C.
Data were acquired using three sets of Omega scans at different Phi settings. The frame width was 0.5° with an exposure time of 5.0 s.

The detailed data collection strategy was as follows:
Detector distance: 40 mm
Detector swing angle (fixed 2 Theta): -20°.

Run	Omega (start)	Omega (end)	Phi	Frames
1	-20.0	160.0	0.0	360
2	-20.0	100.0	120.0	240
3	-20.0	40.0	240.0	120

APEX2 software was used for preliminary determination of the unit cell. Determination of integral intensities and unit cell refinement were performed using SAINT. The integration of the data yielded a total of 6711 reflections to a maximum θ angle of 25.35° (0.83 Å resolution). The constants for the orthorhombic unit cell are a = 5.9724(2) Å, b = 9.0512(2) Å, c = 18.4171(8) Å, V = 995.58(7) $Å^3$. They are based upon the refinement of the XYZ-centroids of 3191 reflections above 20.0 I/σ(I) with 2.21° ≤ θ ≤ 25.25°.
Data were corrected for absorption effects with SADABS using the multiscan technique. The ratio of minimum to maximum apparent transmission is 91.6:100. The average residual for symmetry equivalent reflections is R_{int} = 2.35% and R_σ = 2.32%. XPREP determined the space group to be P 21 21 21, with Z = 4 for the formula unit, $C_{11}H_{10}O_2S$.
The structure was solved with XS and subsequent structure refinements were performed with XL. The final anisotropic full-matrix least-squares refinement on F_o^2 with 129 variables converged at R_1 = 2.89% for the observed data and wR_2 = 7.65% for all data. The goodness-of-fit was 1.046. The largest peak on the final difference electron density synthesis was 0.14 $e^-/Å^3$ and the deepest hole was -0.20 $e^-/Å^3$ with an RMS deviation of 0.04 $e^-/Å^3$. On the basis of the final model, the calculated density is 1.376 g/cm^3 and F(000) = 432.

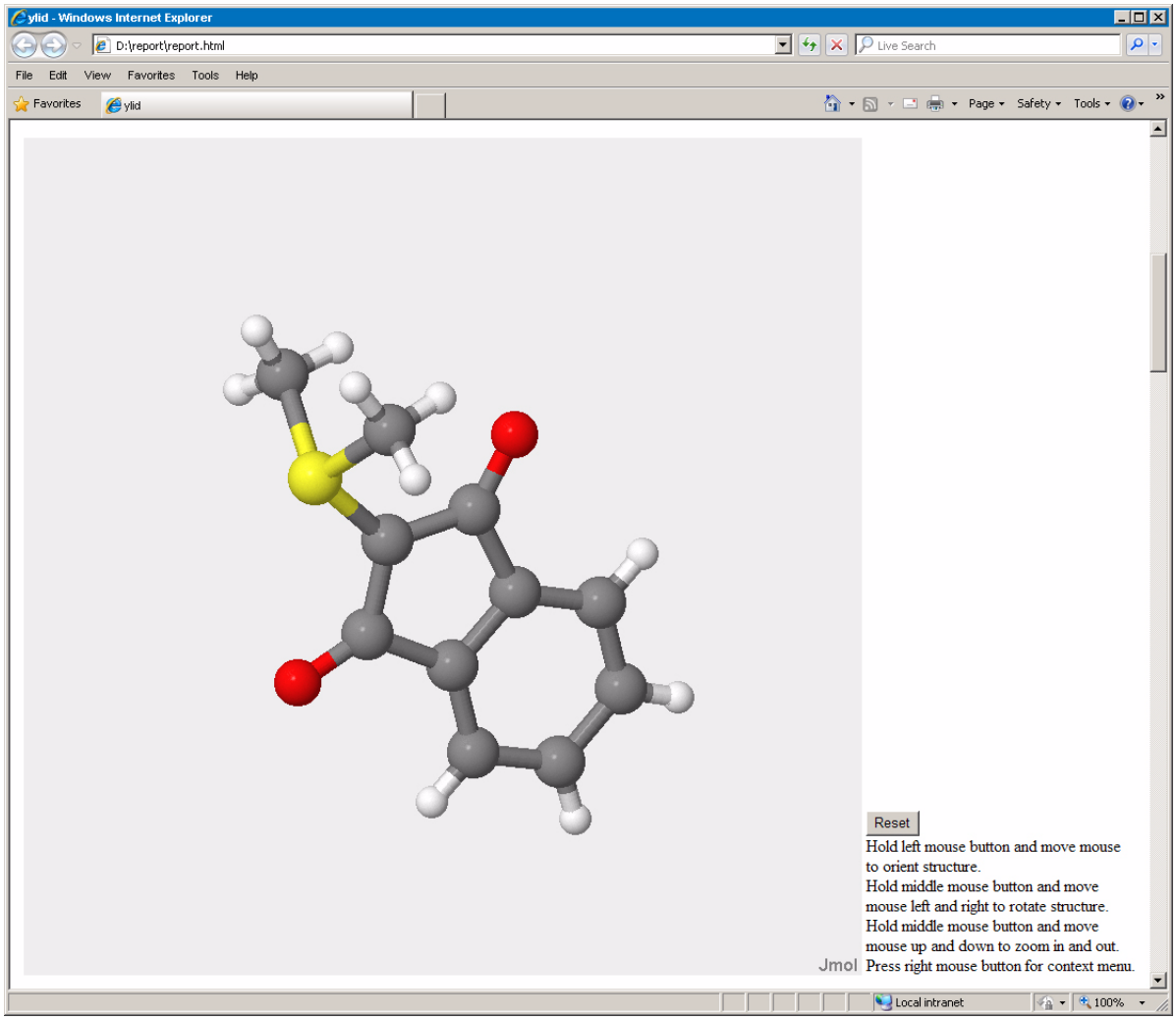
APEX2 Version 2.2 (Bruker AXS Inc., 2007)
SAINT Version 7.34a (Bruker AXS Inc., 2007)
SADABS Version 2007/2 (Sheldrick, Bruker AXS Inc.)
XPREP Version 2005/2 (Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (George M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
XL Version 2008/1 (George M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)

7.1.2 Molecule Viewer Section

The molecule viewer allows for inspection of the structure. The molecule can be rotated and displayed in various modes (e.g., ball-and-stick, space-filling CPK model, molecule surface), and bond lengths, angles, and torsions can be measured.

The molecule viewer uses Jmol, an open-source Java viewer for chemical structures in 3D. Full documentation for Jmol is available at http://jmol.sourceforge.net

Figure 7.2 — Molecule viewer section


ylid - Windows Internet Explorer
D:\report\report.html
Live Search
File Edit View Favorites Tools Help
Favorites
ylid
Page Safety Tools
Reset
Hold left mouse button and move mouse to orient structure.
Hold middle mouse button and move mouse left and right to rotate structure.
Hold middle mouse button and move mouse up and down to zoom in and out.
Press right mouse button for context menu.
Jmol
Local intranet
100%

7.1.3 Detailed Report Section

Crystal Data and Structure Refinement

Figure 7.3 — Crystal data and structure refinement

Table 1. Crystal data and structure refinement for ylid.

Identification code	ylid	
Empirical formula	C11 H10 O2 S	
Formula weight	206.25	
Temperature	300(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 5.9724(2) Å	α = 90°
	b = 9.0512(2) Å	β = 90°
	c = 18.4171(8) Å	γ = 90°
Volume	995.58(7) $Å^3$	
Z	4	
Density (calculated)	1.376 Mg/cm^3	
Absorption coefficient	0.293 mm^{-1}	
F(000)	432	
Crystal size	0.50 x 0.50 x 0.60 mm^3	
Theta range for data collection	2.51 to 25.35°	
Index ranges	-7<=h<=7, -10<=k<=9, -22<=l<=22	
Reflections collected	6711	
Independent reflections	1808 [R(int) = 0.0235]	
Completeness to theta = 25.35°	99.9%	
Absorption correction	Multiscan	
Max. and min. transmission	0.8673 and 0.7941	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1808 / 0 / 129	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0289, wR2 = 0.0743	
R indices (all data)	R1 = 0.0320, wR2 = 0.0765	
Absolute structure parameter	0.01(7)	
Largest diff. peak and hole	0.140 and -0.205	

$R_{int} = \Sigma|F_o^2 - F_o^2(mean)| / \Sigma[F_o^2]$

$R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$

$GOOF = S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$

$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

$w = 1 / [\sigma(F_o^2) + (aP)^2 + bP]$ where P is $[2F_c^2 + Max(F_o^2, 0)] / 3$

Atomic Coordinates and Isotropic Displacement Parameters

Figure 7.4 — Atomic coordinates and isotropic displacement parameters

Table 2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for ylid.

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S1	1903(1)	6814(1)	2596(1)	39(1)
O1	6642(2)	8021(1)	3230(1)	50(1)
O2	1583(3)	4109(1)	3706(1)	52(1)
C1	1652(4)	8768(2)	2710(1)	50(1)
C2	3642(3)	6245(2)	3280(1)	36(1)
C3	5662(3)	6946(2)	3500(1)	37(1)
C4	6422(3)	6143(2)	4174(1)	37(1)
C5	8222(4)	6401(2)	4620(1)	48(1)
C6	8505(4)	5491(3)	5224(1)	57(1)
C7	3505(5)	6760(3)	1773(1)	61(1)
C8	6998(5)	4387(3)	5373(1)	60(1)
C9	5130(4)	4127(2)	4925(1)	51(1)
C10	4901(3)	5018(2)	4320(1)	39(1)
C11	3105(3)	5015(2)	3747(1)	37(1)

Bond Lengths and Angles

Figure 7.5 — Bond lengths and angles

Table 3. Bond lengths (Å) and angles (°) for ylid.

S1-C2	1.7127(18)
S1-C1	1.787(2)
S1-C7	1.792(2)
O1-C3	1.240(2)
O2-C11	1.226(2)
C2-C3	1.423(3)
C2-C11	1.442(3)
C3-C4	1.507(2)
C4-C5	1.372(3)
C4-C10	1.391(3)
C5-C6	1.396(3)
C6-C8	1.372(3)
C8-C9	1.407(3)
C9-C10	1.383(3)
C10-C11	1.505(2)
C2-S1-C1	105.18(9)
C2-S1-C7	106.86(11)
C1-S1-C7	99.88(11)
C3-C2-C11	111.29(16)
C3-C2-S1	126.15(14)
C11-C2-S1	122.41(13)
O1-C3-C2	129.51(17)
O1-C3-C4	124.52(17)
C2-C3-C4	105.95(15)
C5-C4-C10	121.35(17)
C5-C4-C3	130.25(18)
C10-C4-C3	108.38(15)
C4-C5-C6	118.2(2)
C8-C6-C5	120.6(2)
C6-C8-C9	121.7(2)
C10-C9-C8	116.9(2)
C9-C10-C4	121.22(17)
C9-C10-C11	129.40(18)
C4-C10-C11	109.36(15)
O2-C11-C2	130.12(16)
O2-C11-C10	124.91(16)
C2-C11-C10	104.95(15)

Anisotropic Displacement Parameters

Figure 7.6 — Anisotropic displacement parameters

Table 4. Anisotropic displacement parameters ($Å^2x10^3$) for ylid.

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S1	41(1)	35(1)	40(1)	4(1)	-9(1)	-5(1)
O1	45(1)	49(1)	57(1)	13(1)	-2(1)	-11(1)
O2	60(1)	45(1)	52(1)	9(1)	-8(1)	-17(1)
C1	49(1)	38(1)	63(1)	1(1)	-13(1)	9(1)
C2	41(1)	35(1)	34(1)	4(1)	-3(1)	1(1)
C3	36(1)	34(1)	39(1)	-0(1)	2(1)	4(1)
C4	40(1)	36(1)	35(1)	-4(1)	-2(1)	7(1)
C5	43(1)	52(1)	50(1)	-4(1)	-8(1)	6(1)
C6	66(1)	56(1)	48(1)	-7(1)	-24(1)	13(1)
C7	90(2)	54(1)	38(1)	1(1)	4(1)	5(1)
C8	92(2)	48(1)	40(1)	1(1)	-20(1)	14(2)
C9	74(1)	39(1)	39(1)	3(1)	-5(1)	2(1)
C10	51(1)	32(1)	33(1)	-3(1)	-3(1)	5(1)
C11	45(1)	32(1)	35(1)	-1(1)	1(1)	2(1)

Hydrogen Coordinates and Isotropic Displacement Parameters

Figure 7.7 — Hydrogen coordinates and isotropic displacement parameters

Table 5. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for ylid.

	x	y	z	U(eq)
H1A	844	8973	3149	75
H1B	859	9179	2304	75
H1C	3117	9200	2738	75
H5	9224	7161	4521	58
H6	9727	5633	5529	68
H7A	4948	7196	1857	91
H7B	2736	7303	1402	91
H7C	3689	5753	1622	91
H8	7217	3796	5779	72
H9	4096	3389	5031	61

7.1.4 Alerts Section

Below the Detailed Report section is a list of alerts generated by the SMART X2S.

7.2 Using the Data CD with APEX2

The data CD is designed to work with APEX2. To use the SMART X2S data CD with APEX2:

1. Insert the data CD into the computer's drive.
2. If you have a sample open in APEX2, close it.
3. Choose **Sample > Archive > Restore Archive...** from the Menu Bar.

   The "Restore Archived Sample" window opens.
4. Choose the "From CD" tab.
5. The "Using CD Burner:" field should show the drive you wish to restore from. Otherwise, use the **...** button to locate the drive.
6. Click **Get Archive Information from CD**, and insert the archive CD.

   The archive name appears so that you can check it for name conflicts with the existing samples in the Sample Database (shown on the right-hand side of the window). If there is a conflict, you can choose to change the name of the sample in the "Restore As:" field.

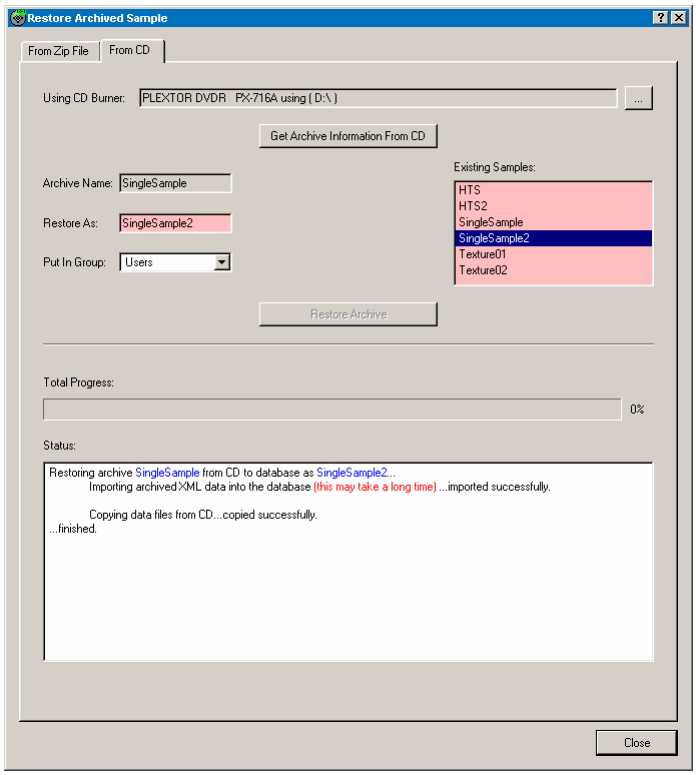
NOTE: If you restore an archived sample using the same name as an already-existing sample, the restored sample will overwrite the already-existing sample in the Sample Database.

7. Choose the appropriate group for the restored archive in the "Put in Group:" drop-down menu.

8. Click **Restore Archive**.

   A progress bar and status data are shown as the software restores the archive.

Figure 7.8 — "Restore Archived Sample" window ("From CD" selected)



When the archive is restored, it can be opened from the **Sample > Open...Sample > Open > Sample...** dialog.

9. Click **Close** to close the "Restore Archived Sample" window.

After "restoring" the sample, you can work with it as you would any other sample in APEX2. For more information on working with APEX2, see M86-Exx078 APEX2 User Manual.

8 SMART X2S Administrator Information

8.1 Access to the SMART X2S' Interior

8.1.1 Administrator Key and Accessories Kit

Administrator Key

The Administrator key is shipped with the SMART X2S. It allows access to the interior of the instrument, including the storage compartment and computer drawer in the lower portion of the unit.

NOTE: One individual should be designated as the "SMART X2S instrument administrator", and this individual should retain the key to prevent unauthorized access to the SMART X2S' interior.

CAUTION

The upper portion of the SMART X2S, which contains the X-ray source, contains no user-serviceable parts and should only be opened by qualified Bruker AXS personnel.

Accessories Kit

The SMART X2S Accessories Kit, shipped with the SMART X2S unit and initially located in the internal accessory compartment, contains the following items:

- Applicable documentation;
- Bruker Spine Pins;
- Blank CD-ROM media;
- Three standard crystals for performance verification:
  - YLID
  - Aspirin
  - Tartaric acid
- A crystal preparation tool;
- Ultraviolet-curing adhesive; and
- An ultraviolet penlight for curing the adhesive.

8.1.2 Opening the SMART X2S Chassis

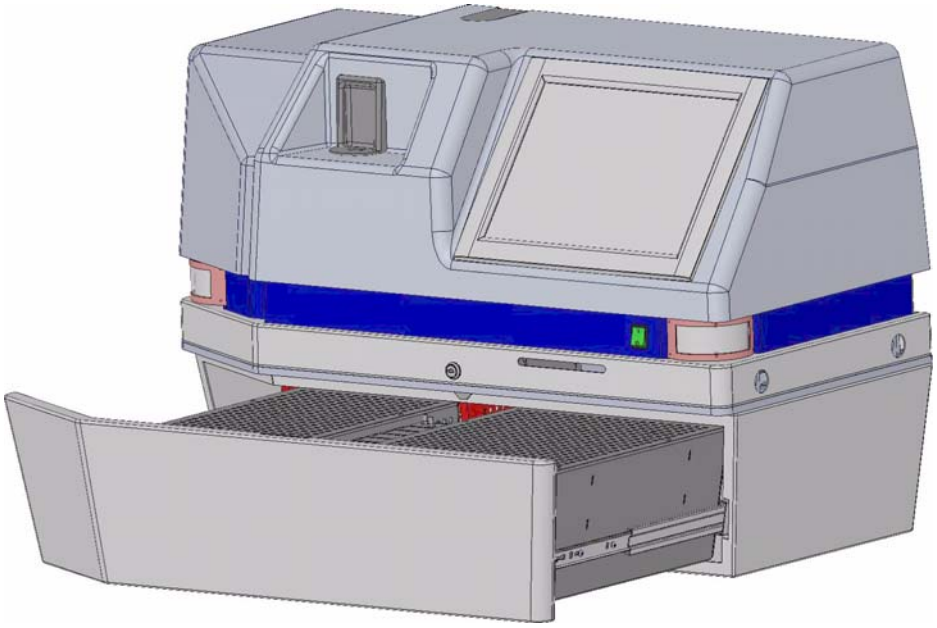
1. Insert the Administrator key and turn it to the 12 o'clock position.

Figure 8.1 — Administrator key at 12 o'clock position

The system's lower drawer will now open, giving you access to the storage compartment, power supplies, and computer.

2. Open the lower drawer by holding it along its edges, pulling up slightly (to make sure that the drawer does not bind against the surface the SMART X2S is sitting on), and pulling outward.

Figure 8.2 — Lower drawer open

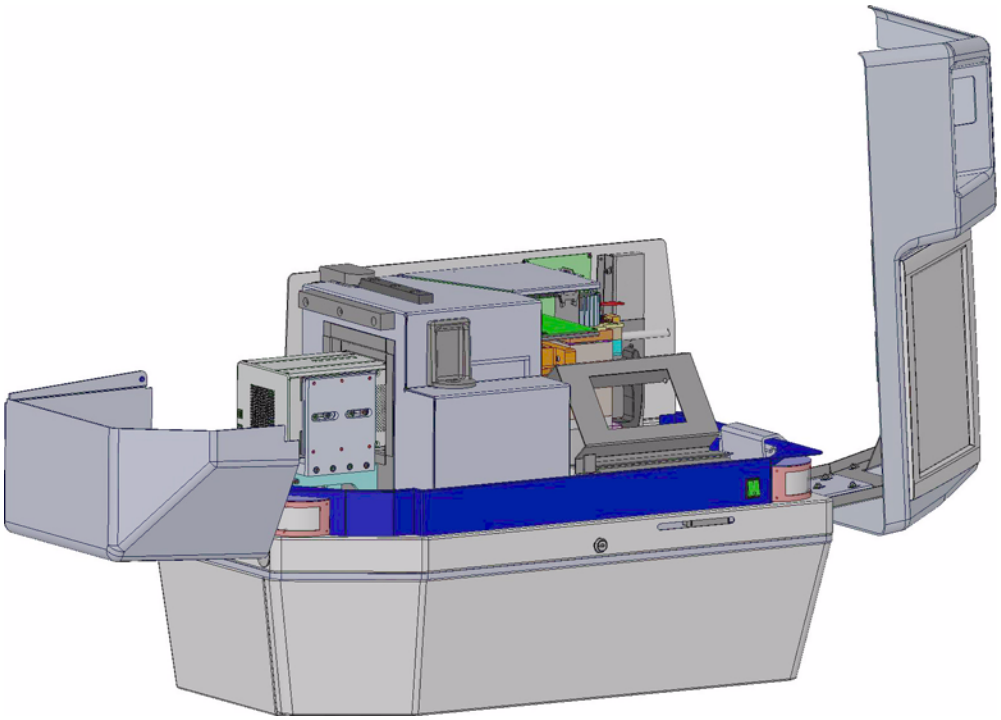


3. If necessary, the hinged upper portion of the system case can be raised for access to the generator, detector, goniostat, sample loader, et al.

CAUTION

Opening or closing the SMART X2S' hinged upper cover creates a pinch hazard. Be aware of this hazard whenever the upper cover is raised.

Figure 8.3 — Hinged upper cover open



8.1.3 SMART X2S Compartments

After opening the lower drawer with the Administrator key, three compartments are visible:

- The leftmost compartment is a storage compartment and typically contains the system's USB keyboard and other miscellaneous items;
- The middle compartment contains a series of power supplies and distribution modules for the SMART X2S' interior components; and
- The rightmost compartment contains the system computer.

8.2 Moving the SMART X2S

8.2.1 Moving the SMART X2S over Short Distances

When moving the SMART X2S over short distances:

- Make sure that the system is powered down and unplugged;
- Make sure that the system's path is clear from its current location to its destination;
- Use a suitable four-wheeled cart or dolly; and
- Attach, lock, and use the system's removable carrying handles.

8.2.2 Crating the SMART X2S for Shipping

Moving the SMART X2S to its Staging Location

1. Move the SMART X2S from its installed location to a safe staging location where it can be attached to its shipping skid and dressed for shipment.

Attaching the Outriggers

1. Elevate the SMART X2S (e.g., on a cart), to allow access to the right and left sides of the bottom of the unit. The sides have screw holes that will be used to attach the wooden “outriggers” (that attach to the shipping skid).

Figure 8.4 — Underside of SMART X2S: holes for outrigger

2. Attach the outriggers to the bottom of the SMART X2S with two M10×30 screws, with washers. Tighten them just to the point where they are secure, but can be knocked into position.

Figure 8.5 — Outrigger

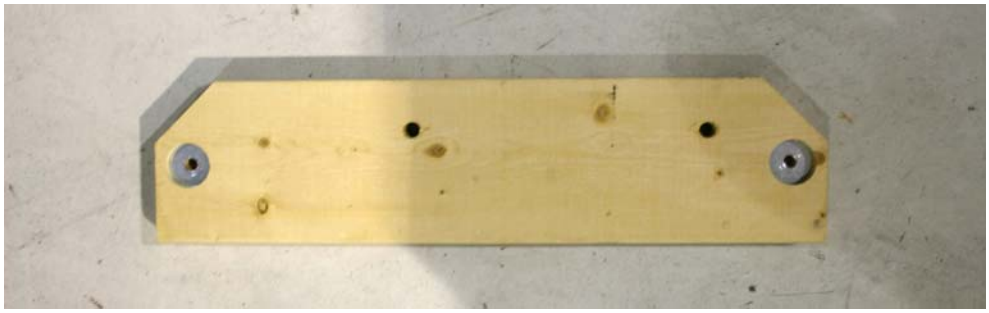
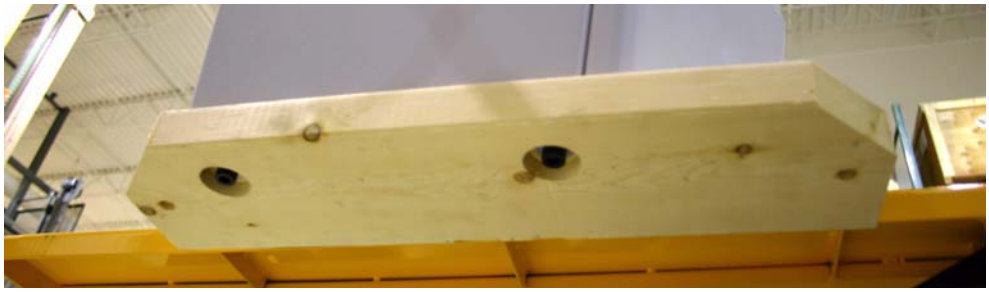


Figure 8.6 — Underside of SMART X2S: outrigger attached



Moving the SMART X2S onto its Shipping Skid

The SMART X2S' wooden outriggers attach to the shipping skid with four 9/16" bolts.

1. Position the skid so that the SMART X2S can be moved onto it as easily as possible (the skid does not have a special front/back orientation).

Figure 8.7 — Shipping skid with four 9/16" bolts and wrench

2. With a person on each side, move the SMART X2S directly down onto the skid.

Figure 8.8 — SMART X2S on shipping skid

3. Attach the SMART X2S' outriggers to the skid with the four 9/16" bolts. It may be necessary to move the SMART X2S around on top of the skid to get the outriggers' holes and the skid's holes to line up.

Dressing the SMART X2S for Shipping

After the SMART X2S is securely attached to the skid, add the protective plastic cover and additional components.

1. Slide the protective plastic cover over the SMART X2S.

Figure 8.9 — Plastic cover

2. Wrap the carrying handles in bubble wrap and place them along the rear of the SMART X2S chassis.

Figure 8.10 —Carrying handles along rear

3. Include any extra items to be shipped with the SMART X2S by bagging them and placing them along the top of the unit (these may include the Accessory kit, the USB keyboard, and any documentation). These items will be placed down along the sides of the unit when the crate is screwed together.

Figure 8.11 —Extra items

Screwing the Crate Together

1. Use a screw gun and wood screws to attach the sides of the crate.
2. Move the additional materials from the top of the SMART X2S down into the bottom of the crate on one of the sides.
3. Finally, use the screw gun and wood screws to attach the top of the crate.

8.2.3 Uncrating the SMART X2S

Moving the Crate to a Staging Location

1. Begin by moving the crate to a staging location, clear on all sides, where the SMART X2S can be safely uncrated and moved.

Unscrewing the Crate

1. Use a screw gun to remove the top and sides of the crate.

Removing the Shipping Materials

1. Remove any miscellaneous items (e.g., documentation, accessory kit) from the inside of the crate.
2. Remove and unpack the four carrying handles that are included with the unit.
3. Remove the plastic shipping cover.

Removing the Unit from the Skid

1. Four bolts attach the SMART X2S' two wooden "outriggers" to the skid. Remove them.
2. Install the carrying handles by inserting them and rotating them to their locking positions.
3. Raise the SMART X2S and turn it 90°, so that the two "outriggers" are elevated off the ground.

Figure 8.12 —Turning the SMART X2S 90° on its skid for removal of outriggers

4. Unscrew and remove the "outriggers".

Moving the Unit to its Installed Location

1. Use the carrying handles to move the unit to its installed location.

NOTE: Observe proper safety and lifting precautions when moving the unit.

2. Retain all shipping materials in case the unit must be returned to Bruker.

8.3 Preventive Maintenance and Inspections

8.3.1 Cleaning the SMART X2S

The SMART X2S' exterior panels may be cleaned with a damp cloth. Do not use soap or aggressive cleansing agents.

In order to avoid damage to the touchscreen, the use of sharp objects such as styluses should be avoided. To clean the touchscreen, avoid the use of abrasives or aggressive solvents; only use a soft, damp cloth with a mild detergent if necessary.

To ensure adequate airflow through the SMART X2S, periodically check that the rear ventilation holes are clear of dust and debris.

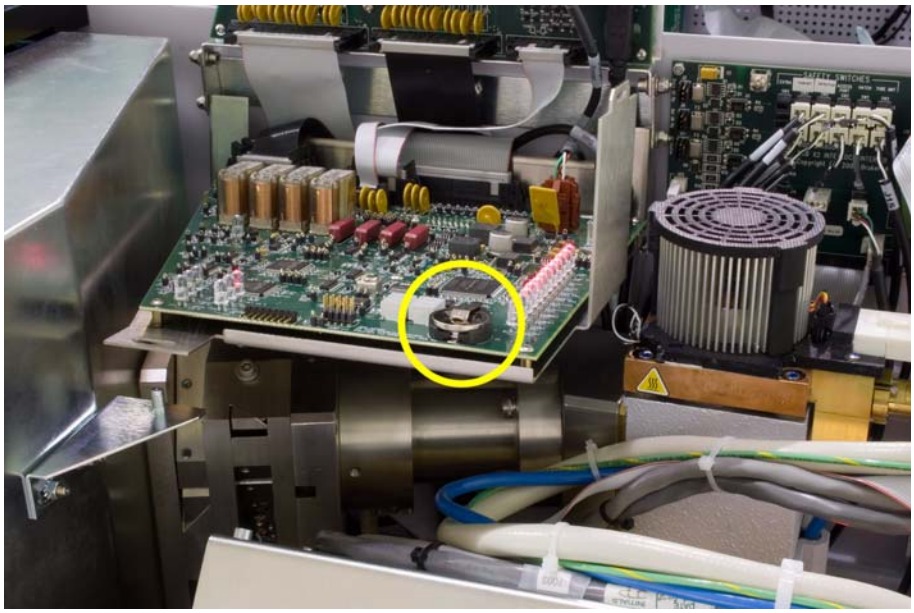
8.3.2 Replacing the Lithium Battery

The SMART X2S' goniostat/interlock PCB uses a lithium battery. To ensure that the battery does not fail, replace it once every 2 years as part of a biannual preventative maintenance procedure. The battery is available from Bruker AXS as part number 122-004600.

To replace the battery:

1. Use the Administrator key to open the SMART X2S, and lift off the top cover.
2. Locate the battery in socket J16 on the goniostat/interlock PCB (i.e., the lower of the two circuit boards immediately to the right-hand side of the radiation shield enclosure).

Figure 8.13 —Lithium battery location



3. Remove the battery from under the contact clip. A capacitor will preserve the board's memory while there is no battery in the socket.
4. Place the new battery into the socket, positive (+) side up, under the contact clip.

8.3.3 Surveying the SMART X2S for Radiation Leakage

The SMART X2S should be surveyed for radiation leakage and stray radiation as a closed-beam X-ray diffraction system in accordance with the following documents:

- Guide for submission of information on Analytical X-ray Equipment required pursuant 21 CFR 1002.10.
- National Bureau of Standards Handbook III Radiation Safety for X-ray Diffraction and Fluorescence Analysis Equipment.

CAUTION

Radiation surveys should only be performed by—or under the immediate supervision of—qualified Bruker AXS personnel.

X-ray Emission

1. Perform the X-ray emission survey with the X-ray tube to be supplied with the instrument, operated at a power level of 50kV and 1 mA to produce the maximum X-ray exposure. (Reduce the mA as necessary so as not to exceed the maximum rated power of the tube.) The test shall be conducted with the supplied optics.

CAUTION

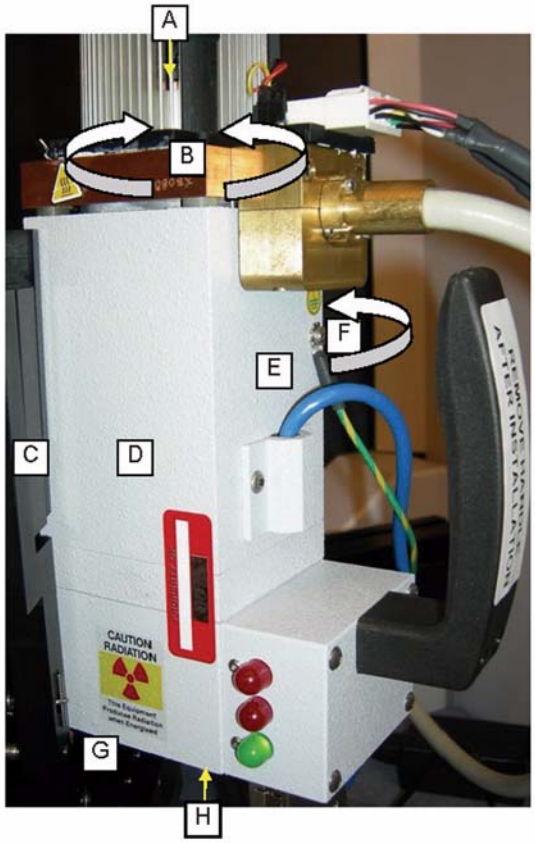
Individuals performing the survey should wear leaded safety glasses as a precaution. Dosage in excess of 2.5 mR/hr may be hazardous to the eyes.

Radiation Leakage

1. Close the shutter.
2. Survey the entire tube housing with the Geiger counter at a distance of 50 mm from the surface of the tube housing to determine areas of high intensity radiation emission.
3. When a radiation emission area has been located, measure the specific emission averaged over one square cm with the Victoreen 440 RF/C ionization detector at a distance of 50 mm from the surface of the tube housing.
4. Record the location and measured intensity of leakage radiation on the diagram. The leakage radiation shall not exceed 0.5 mR/hr.

Tube Shield Radiation Leakage Survey Form

Tube Shield Serial #: _____



	A	B	C	D	E	F	G	H
Survey Meter								
Ion Chamber								

SURVEYED BY: _____ DATE: _____

Stray Radiation

1. Use the “SMART X2S Admin” application (on the SMART X2S Service CD) to open the X-ray shutter.

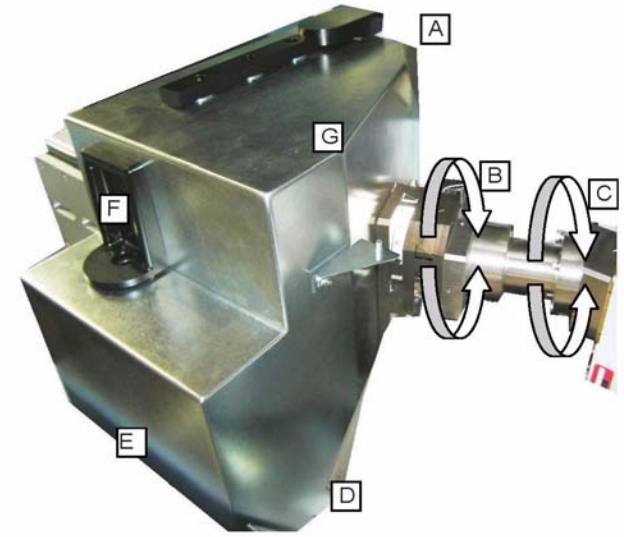
CAUTION

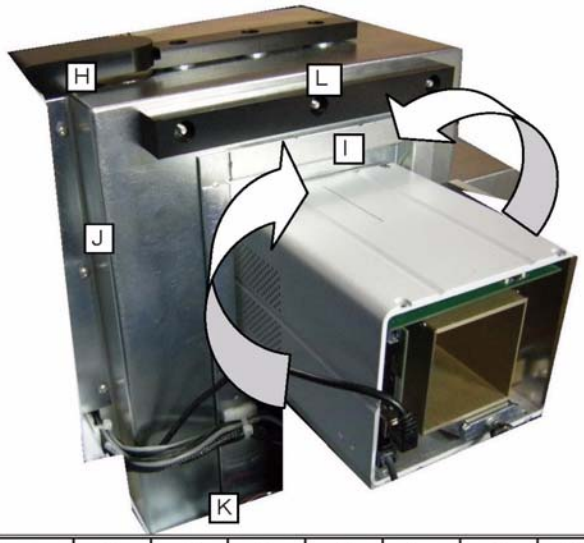
If you do not have the SMART X2S Service CD available, contact Bruker AXS. Do not attempt to open the X-ray shutter in any other way unless specifically directed by Bruker AXS personnel.

2. Survey the entire SMART X2S cabinet with the Geiger counter at a distance of 50 mm from the surface to determine areas of high intensity radiation emission.
3. When a radiation emission area has been located, measure the specific emission averaged over 100 square cm with the Victoreen RF/C ionization detector at a distance of 50 mm from the surface of the goniometer cabinet.
4. Record the location and measured intensity of stray radiation on the diagram. The stray radiation shall not exceed 0.5 mR/hr.

System Cabinet Radiation Survey Form

SMART X2S System Serial #: _____





	A	B	C	D	E	F	G	H	I	J	K	L
Survey Meter												
Ion Chamber												

SURVEYED BY: _____ DATE: _____

8.4 The SMART X2S' Archival and Deletion Routine

The data CD, burned at the end of data collection, is a copy of a folder on the SMART X2S' internal hard drive. An instrument administrator can easily retrieve any sample in the SMART X2S' history of operation—until the hard drive becomes nearly full.

Once the hard drive is nearly full, the system automatically removes files each time a new sample is collected. It goes through each sample folder—oldest to newest—and removes enough frame files to ensure that a new sample has enough space for data collection. If the free space is still insufficient, the system goes through each sample folder (again, oldest to newest) to remove all remaining traces of the sample until there is enough space for the new sample's data.

Typically, this means that, when the SMART X2S' hard drive is nearly full, it removes the oldest sample to make room for the newest.

The number of samples that can be stored is dependent upon the hard drive's storage capacity, and is subject to change without notice.

8.5 Remote Access to the SMART X2S' Frames Directory

NOTE: The SMART X2S does not have any intrinsic virus protection software installed, and is therefore vulnerable to external network threats. Protecting your SMART X2S from malware is your responsibility, and Bruker AXS is not accountable for any inoperability or data loss as a result of connectivity to a network.

8.5.1 Connect the Computer to the SMART X2S

The preferred method of remote access to the data on your SMART X2S' hard drive is to use an isolated/private network configuration. This consists of a computer with two separate network cards, a router with DHCP, and the SMART X2S.

The SMART X2S is set up to obtain an IP address automatically when connected to a DHCP-enabled intranet connection.

1. Use a standard network cable to connect the computer's secondary network interface card to the router.
2. Use a standard network cable to connect the Ethernet port on the SMART X2S' rear to the router.
3. Plug the router's power supply into a standard outlet.

8.5.2 Check that the SMART X2S Has a Dynamic IP Address

NOTE: Before checking, be sure that the USB keyboard is connected.

1. Type [Ctrl]+[Alt]+[Del].
2. Choose **Task Manager**.
3. Click the **New Task...** button, and type `cmd`.
4. At the command prompt, type `ipconfig` to reveal the IP address assigned to the SMART X2S.

8.5.3 Connect the SMART X2S to the Isolated Private Network

Map a network drive to the SMART X2S' D:\frames\ directory by following these steps:

1. On the Desktop, right-click the "My Computer" icon and choose **Map Network Drive**.

   The "Map Network Drive" window opens.

2. Set the network drive options:

   2.1. In the "Drive:" menu, choose an available drive letter.
   2.2. In the "Folder:" menu, enter the following: `\\smartx2s\frames\`
   2.3. Activate the **Reconnect at Logon** checkbox.

3. Set the connection options:

   3.1. Click the words different user name.
   The "Connect As…" window opens.
   3.2. Enter a user name: `smartx2s\Administrator`
   3.3. Enter a password: `Bruker`
   3.4. Click **OK** to exit the "Connect As…" window.

4. Click **Finish** to create the mapped network drive.

8.6 Connecting to WebEx

WebEx is a network technology that allows remote control of computer systems over the internet.

In the event of a problem with the SMART X2S, Bruker AXS Service personnel can remotely control, diagnose, and even repair your SMART X2S unit using WebEx.

NOTE: Before connecting the system to WebEx, Contact Bruker AXS Service by phone, and follow the Service Engineer's instructions. Make sure that the system is connected to the internet via the rear Ethernet port.

To use WebEx with the SMART X2S:

1. Insert the SMART X2S Service CD into the CD writer while the system is booting. This CD should be present in the lower drawer's right-hand compartment.

   After the boot process, the SMART X2S Control Panel application will appear.

2. In the SMART X2S Control Panel application, click the **WebEx** button.

   Internet Explorer opens and contacts https://bruker-axs.webex.com/sc to begin the WebEx session.

8.6.1 Connecting to WebEx without a SMART X2S Service CD

If the SMART X2S Service CD is not available, contact Bruker AXS Service.

8.7 Updating the SMART X2S Software

8.7.1 Preparing for the Software Update

1. Power down the SMART X2S by flipping the green power switch.

Figure 8.14 —Power switch

2. Use the Administrator key to unlock the lower drawer.

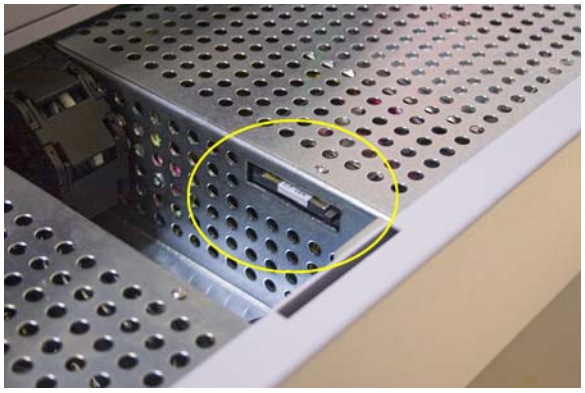
Figure 8.15 —Using the Administrator key

3. Pull out the lower drawer.

Figure 8.16 —Lower drawer pulled out

4. Some SMART X2S models have the Compact Flash card slot on the inside of the computer compartment. Look for the Compact Flash card slot on the computer compartment's left-hand side.

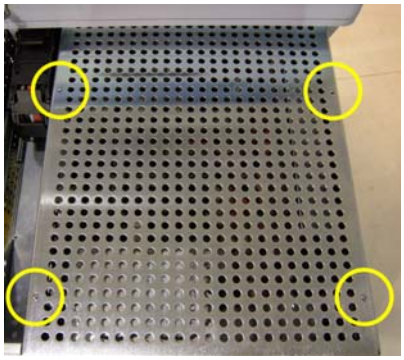
Figure 8.17 —Computer compartment left-hand side (Compact Flash card slot present)



- **If the slot is visible**, proceed to Section 8.7.2.
- **If the slot is not visible**, open the computer compartment:

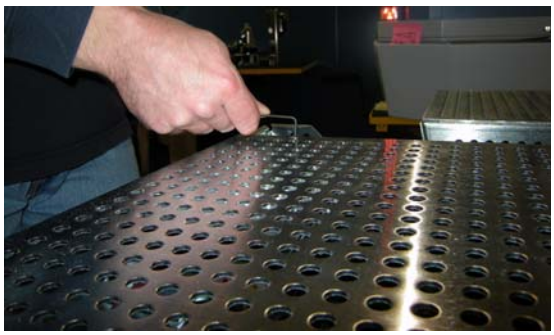
4.1. Locate the four hex bolts in the computer compartment's top cover.

Figure 8.18 —Computer compartment top cover: locations of hex bolts



4.2. Remove the four hex bolts using a 2-mm hex wrench.

Figure 8.19 —Removing the hex bolts



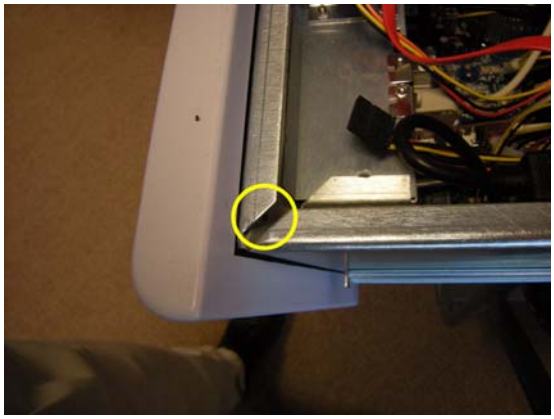
4.3. Lift the top cover off the computer compartment, and set it aside.

Figure 8.20 —Removing the top cover

4.4. Remove the 4-mm hex bolts in the top left-hand and top right-hand corners of the drawer.

Figure 8.21 —Top left-hand hex bolt

Figure 8.22 —Top right-hand hex bolt



4.5. Separate the drawer from the computer chassis, and set it aside.

Figure 8.23 —Removing the drawer from the computer chassis

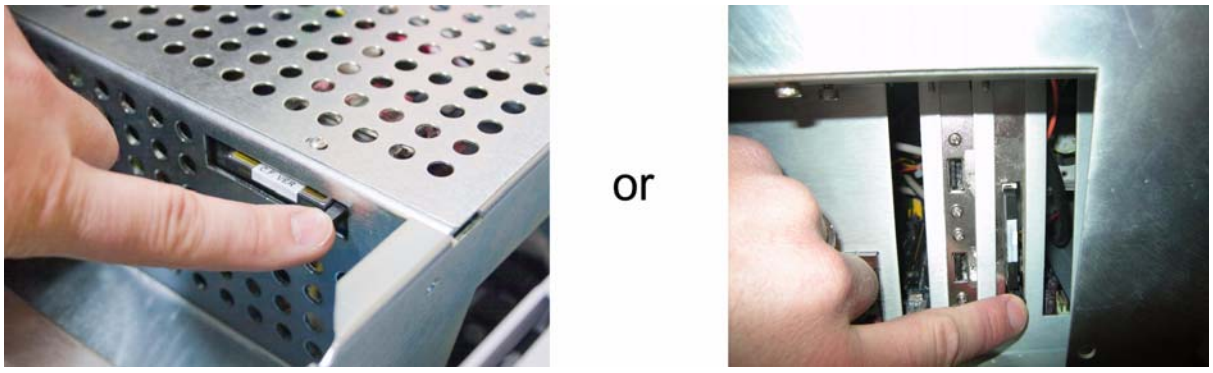
4.6. Remove the drawer panel from the computer compartment.

8.7.2 Replacing the Compact Flash Card

1. Remove the Compact Flash card.

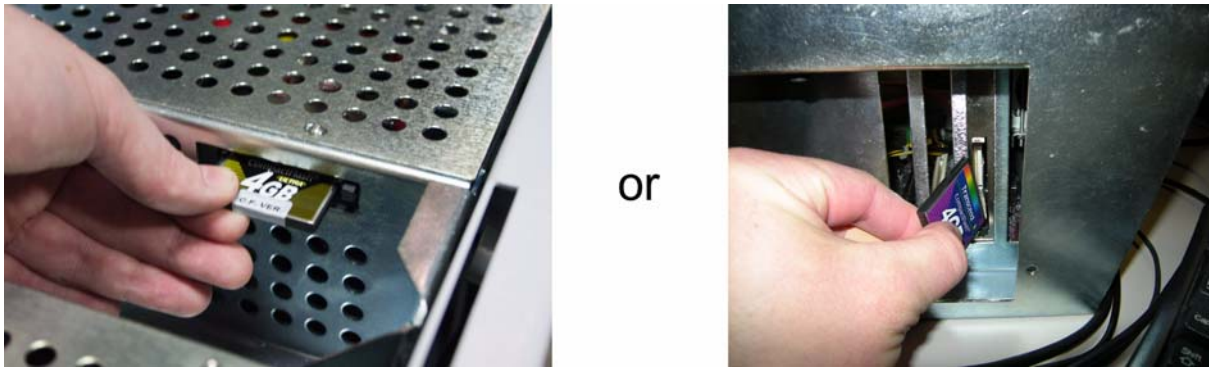
    1.1. Press the small black eject button next to the card.

Figure 8.24 —Ejecting the Compact Flash card



    1.2. Pull the card out of the slot and set it aside.

Figure 8.25 —Removing the Compact Flash card



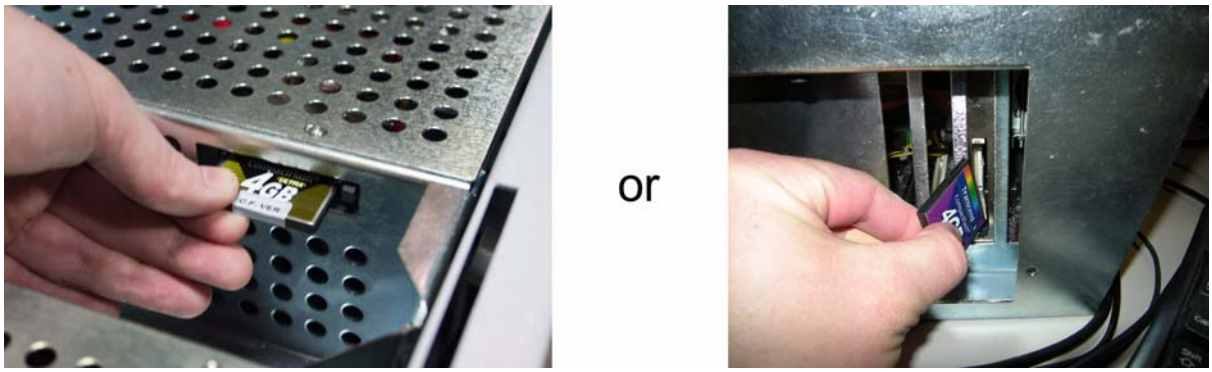
2. Insert the new Compact Flash card.

    2.1. Locate the new Compact Flash card.

Figure 8.26 —New Compact Flash card (your version number may vary)

2.2. Insert the Compact Flash card into its slot, making sure that the card orientation is the same as shown.

Figure 8.27 —Inserting the Compact Flash card



8.7.3 After Updating the Software

1. If your Compact Flash card slot is on the inside of the computer compartment, close up the computer compartment:
    1.1. Using the 4-mm hex wrench, attach the drawer to the computer chassis by replacing the two hex bolts that were removed in Section 8.7.1, step 4.
    1.2. Using the 2-mm hex wrench, replace the computer compartment top cover that was removed in Section 8.7.1, step 4.
2. Push in the drawer, and lock it using the Administrator key.
3. Power on the SMART X2S by flipping the green power switch.

Figure 8.28 —Power switch

The instrument powers up and the computer boots. The software will automatically detect that a new card is present, perform some configuration steps, and then restart the instrument again.

Figure 8.29 —SMART X2S startup: “New CF card detected” screen

After the computer has restarted the second time, the software update process is finished and the system is ready to use.

8.8 Consumable Items

Part Number	Quantity	Description
070-003200	2	Replaceable fuse, 3.15A, 250V, SLO-BLO
122-004600	1	Replaceable battery, lithium, Panasonic CR2032

8.9 CE Declaration of Conformity

Figure 8.30 —SMART X2S CE Declaration of Conformity

Bruker AXS Inc.
5465 East Cheryl Parkway
Madison, WI 53711-5373
Tel. +1 (608) 276-3000
Fax +1 (608) 276-3006
info@bruker-axs.com
www.bruker-axs.com

DECLARATION OF CONFORMITY

Manufacturer's Name: Bruker AXS Inc.

Manufacturer's Address: 5465 East Cheryl Parkway
Madison, WI 53711-5373 USA

Declares that the product:

Product Name: SMART X2S

Model Number: 882-030500

Conforms to the following product specifications:

Safety: EN 61010-1:2001 (2nd Edition)

EMC: EN 55011:1998 with Amendment A1:1999, Group 1, Class A, for ISM Equipment
EN 61326-1:2006 using IEC 61000-4-2:2001, -3:2002, -4:2004, -5:2001, -6:2003 and -11:2004
EN 61326 using EN 61000-3-2:2000, A2:2005
EN 61326 using EN 61000-3-3:1995, A1:2001, A2:2005

Year in which the CE marking is affixed: 2009

Kline Wilkins
Sr. V.P. Global Operations

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